=> file req

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STRUCTURE FILE UPDATES: 6 APR 2003 HIGHEST RN 501901-52-6
DICTIONARY FILE UPDATES: 6 APR 2003 HIGHEST RN 501901-52-6

=> d his

(FILE 'HOME' ENTERED AT 09:49:12 ON 07 APR 2003)

FILE 'REGISTRY' ENTERED AT 09:49:51 ON 07 APR 2003 ACTIVATE SZEKELY306/A

L1 STR

L2 SCR 1771 L3 SCR 1312

L4 9203 SEA FILE=REGISTRY SSS FUL L1 AND L3 AND L2

FILE 'LREGISTRY' ENTERED AT 09:50:56 ON 07 APR 2003

L5 STR

FILE 'REGISTRY' ENTERED AT 10:13:28 ON 07 APR 2003 L6 1 S L5 SSS SAM SUB=L4

FILE 'LREGISTRY' ENTERED AT 10:14:36 ON 07 APR 2003 L7 STR L6

FILE 'REGISTRY' ENTERED AT 10:22:07 ON 07 APR 2003

L8 50 S L7 SSS SAM SUB=L4

L9 960342 S PMS/CI

L10 2 S L8 NOT L9

L11 4 S L8 AND (0-10/CL OR 0-10/BR)

FILE 'LREGISTRY' ENTERED AT 10:36:51 ON 07 APR 2003 L12 STR L5

FILE 'REGISTRY' ENTERED AT 11:31:59 ON 07 APR 2003

FILE 'LREGISTRY' ENTERED AT 11:33:21 ON 07 APR 2003

FILE 'REGISTRY' ENTERED AT 11:34:36 ON 07 APR 2003 L14 183 S L12 SSS FULL SUB=L4 SAVE SZEK306A/A L14

FILE 'LREGISTRY' ENTERED AT 11:36:37 ON 07 APR 2003

```
FILE 'HCA' ENTERED AT 11:38:30 ON 07 APR 2003
T.15
           224 S L14
    FILE 'REGISTRY' ENTERED AT 11:39:12 ON 07 APR 2003
L16
            148 S L14 NOT 0-10/NR
L17
             9 S L16 AND 1-10/N
L18
            139 S L16 NOT L17
L19
            120 S L18 AND 1/NC
L20
             0 S L19 AND (1-10/F OR 1-10/CL OR 1-10/BR)
     FILE 'HCA' ENTERED AT 11:46:28 ON 07 APR 2003
L21
           183 S L19
     FILE 'REGISTRY' ENTERED AT 11:48:05 ON 07 APR 2003
L22
              SCR 1918
L23
           119 S L19 NOT 0-10/M
     FILE 'HCA' ENTERED AT 11:49:14 ON 07 APR 2003
L24
            183 S L23
L25
            180 S L24 AND 1907-2001/PY
L26
            175 S L24 AND 1907-2000/PY
L27
            170 S L24 AND 1907-1999/PY
L28
         344008 S 37/SC,SX
L29
              7 S L27 AND L28
L30
            163 S L27 NOT L29
     FILE 'LREGISTRY' ENTERED AT 12:00:19 ON 07 APR 2003
     FILE 'HCA' ENTERED AT 12:01:25 ON 07 APR 2003
        827641 S 36/SC, SX OR 38/SX, SC OR 39/SC, SX
L31
              7 S L27 AND L31
L32
L33
            14 S L29 OR L32
           156 S L30 NOT L33
L34
         27814 S HEAT? (N) STABIL?
L35
             1 S L34 AND L35
L36
L37
              5 S L33 AND L35
L38
             15 S L33 OR L36 OR L37
            155 S L34 NOT L38
L39
                SAVE L39 SZEK306AA/A
    FILE 'LREGISTRY' ENTERED AT 12:04:57 ON 07 APR 2003
1.40
               STR L7
    FILE 'REGISTRY' ENTERED AT 12:09:28 ON 07 APR 2003
L41
               SCR 1838
             50 S L40 NOT L22 SSS SAM SUB=L4
L42
L43
               SCR 2036
             50 S L40 NOT (L22 OR L43) SSS SAM SUB=L4
L44
               SCR 1992
L45
             50 S L40 NOT (L22 OR L45) SSS SAM SUB=L4
L46
             4 S L46 AND 1-20/X
L47
             24 S L46 AND 1-2/NC
L48
               E POLYVINYL CHLORIDE/CN
L49
             1 S E3
               E POLYVINYLIDENE CHLORIDE/CN
               E POLYVINYL BROMIDE/CN
               E POLYETHYLENE/CN
L50
              1 S E3
               E RUBBER/CN
```

```
L51
               1 S E3
                E POLYCHLOROPRENE/CN
T.52
               1 S E3
                 E POLYSTYRENE/CN
L53
               1 S E3
T.54
               2 S L49 OR L52
     FILE 'HCA' ENTERED AT 12:19:21 ON 07 APR 2003
L55
           91057 S L54
           10523 S L50(L) (HALOGEN? OR FLUOR? OR CHLORI? OR BROMID?)
L56
               O S L51(L) (HALOGEN? OR FLUOR? OR CHLORI? OR BROMID?)
L57
            6500 S L53(L) (HALOGEN? OR FLUOR? OR PERFLUORO? OR CHLOR? OR PERCHLOR
L58
L59
               O S L51(L) (HALOGEN? OR FLUOR? OR PERFLUORO? OR CHLOR? OR PERCHLOR
L60
          103905 S L55 OR L56 OR L58 OR L51
     FILE 'LCA' ENTERED AT 12:23:35 ON 07 APR 2003
            389 S POLYVINYLCHLORID? OR PVC OR (POLYVINYL# OR POLYETH? OR STYREN
L61
     FILE 'REGISTRY' ENTERED AT 12:28:41 ON 07 APR 2003
L62
              50 S L40 NOT (L22 OR L45) SSS SAM SUB=L4
              50 S L40 NOT L45 SSS SAM
L63
                                         SUB=L4
L64
              50 S L40 NOT L45 SSS SAM
                                          SUB=I.4
L65
           1141 S L40 NOT L45 SSS FULL
                                         SUB=1.4
                 SAVE L65 SZEK306B/A
     FILE 'HCA' ENTERED AT 12:30:51 ON 07 APR 2003
L66
           1398 S L65
     FILE 'REGISTRY' ENTERED AT 12:30:58 ON 07 APR 2003
L67
               0 S L65 AND (L49 OR L52)
L68
               0 S L65 AND (L49 OR L50 OR L53)
     FILE 'HCA' ENTERED AT 12:34:09 ON 07 APR 2003
L69
         113363 S L61
L70
         141867 S L69 OR L55 OR L58 OR L60 OR L51
             201 S L66 AND L70
96 S L71 AND 1907-2000/PY — Publication Year
REGISTRY' ENTERED AT 12:37:24 ON 07 APR 2003 1907-2000
L71
            101 S L66 AND L70
L72
     FILE 'LREGISTRY' ENTERED AT 12:37:24 ON 07 APR 2003
     FILE 'REGISTRY' ENTERED AT 12:37:36 ON 07 APR 2003
     FILE 'HCA' ENTERED AT 12:38:28 ON 07 APR 2003
L73
             76 S L72 AND (L28 OR L31)
L74
          51123 S HEAT(2N) (STABL? OR STABIL? OR DEGRAD?)
L75
             41 S L73 AND L74
L76
             39 S L75 NOT (L38 OR L39)
     FILE 'REGISTRY' ENTERED AT 12:46:21 ON 07 APR 2003
L77
           1141 S L65 NOT L39
L78
           1135 S L65 NOT L14
                                     e Limited number of
on 07 APR 2003 Components
L79
            943 S L78 AND 1-3/NC
L80
            644 S L78 AND 1-2/NC
    FILE 'HCA' ENTERED AT 12:48:49 ON 07 APR 2003
L81
           1358 S L79
L82
           1265 S L80
L83
             91 S L82 AND L61
L84
             80 S L82 AND L60
1.85
             99 S L83 OR L84
```

```
L86
              46 S L85 AND L74
L87
          831285 S L85 AND STABL? OR STABIL?
L88
              63 S L85 AND (STABL? OR STABIL?)
L89
              12 S L83 AND PLASTICI?
L90
              53 S L86 OR L89
L91
               5 S L86 AND PLASTICI?
L92
              12 S L89 OR L91
L93
              67 S L81 AND HEAT(2N)(STABL? OR STABIL? OR DEGRAD?)
1.94
              5 S L93 AND PLASTICI?
L95
              12 S L89 OR L91 OR L94
              81 S L81 AND (HEAT OR THERMAL) (2N) (STABL? OR STABIL? OR DEGRAD?)
L96
              6 S L96 AND PLASTICI?
L97
L98
              12 S L95 OR L97
L99
              41 S L86 NOT L98
     FILE 'LREGISTRY' ENTERED AT 13:00:06 ON 07 APR 2003
     FILE 'REGISTRY' ENTERED AT 13:00:40 ON 07 APR 2003
=> d que stat L14
                 STR
   11
                  12
                   c <
                   S 6
                  E1
NODE ATTRIBUTES:
HCOUNT IS E1
                  ΑТ
                        6
CONNECT IS E1 RC AT
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS
STEREO ATTRIBUTES: NONE
L2
                SCR 1771
L3
                SCR 1312
L4
           9203 SEA FILE=REGISTRY SSS FUL L1 AND L3 AND L2
L12
                STR
                                   Peter,
This is for Claum 1
       12
               13
        0
               0
        1
               1
           6
Ak \sim 0 \longrightarrow C \sim Ak \sim C \longrightarrow O \sim Ak
    4
       5
                   8
```

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

HS 14

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

SEARCH TIME: 00.00.12

183 SEA FILE=REGISTRY SUB=L4 SSS FUL L12

100.0% PROCESSED 4400 ITERATIONS

F.1

183 ANSWERS

=> d que stat L65 L111 12 0 С S 6

NODE ATTRIBUTES:

HCOUNT IS E1 ΑT 6 CONNECT IS E1 RC AT DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS

STEREO ATTRIBUTES: NONE

L2 SCR 1771 L3 SCR 1312

L49203 SEA FILE=REGISTRY SSS FUL L1 AND L3 AND L2 L40 STR

12 13 0 0 HS--- Ak-- O--- C-- Ak-·-- 0· ^Ak~^SH 11 3 96 8 9 10 0 0 HS ~ Ak ~ C = O ~ Ak ~ O = C ~ Ak ~ SH 14 15 16 17 018 19 20 21 22

VAR G1=6/18

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 23

L45

STEREO ATTRIBUTES: NONE SCR 1992

L65

1141 SEA FILE=REGISTRY SUB=L4 SSS FUL L40 NOT L45

100.0% PROCESSED 1599 ITERATIONS

1141 ANSWERS

SEARCH TIME: 00.00.01

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FILE COVERS 1907 - 3 Apr 2003 VOL 138 ISS 15 FILE LAST UPDATED: 3 Apr 2003 (20030403/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d L38 1-15 cbib abs hitind hitstr

publication year

- L38 ANSWER 1 OF 15 HCA COPYRIGHT 2003 ACS

 128:205227 Diisocyanate derivatives and their use in making optical lenses.

 Kawauchi, Keiya; Suzuki, Yoshiyuki; Kobayashi, Seiichi; Imai, Masao;

 Fujii, Kenichi (Mitsai Toatsu Chemicals, Inc., Japan). Jpn. Kokai Tokkyo

 Koho JP 10045707 A2 19980217 Heisei, 8 pp. (Japanese). CODEN:

 JKXXAF. APPLICATION: JP 1996-200400 19960730.

 AB Sulfur-contg. diisocyanate deriv. OCNR(R')nNCO (R = ethylene, propylene,
- AB Sulfur-contg. diisocyanate deriv. OCNR(R')nNCO (R = ethylene, propylene, 2-thiapropylene; R' = methylthio, methylthiomethylthio; n = 1-3) is synthesized. An optical resin compn. having high refractive index comprises the diisocyanate and at least one polythiol compd. The resin compn. can be polymd. to provide optical lenses.
- IC ICM C07C323-45
 - ICS C08G018-77; G02B001-04
- CC 35-2 (Chemistry of Synthetic High Polymers) Section cross-reference(s): 23, 38
- IT 17660-58-1P, Diethyl 2,3-dimercaptosuccinate 56078-31-0P
 90647-87-3P 204063-03-6P 204063-04-7P 204063-05-8P 204063-06-9P
 204063-07-0P 204063-08-1P 204063-09-2P
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT
 (Reactant or reagent)

(prepn. of diisocyanate derivs. for making optical lenses)

- IT 17660-58-1P, Diethyl 2,3-dimercaptosuccinate
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT
 (Reactant or reagent)
 - (prepn. of diisocyanate derivs. for making optical lenses)
- RN 17660-58-1 HCA
- CN Butanedioic acid, 2,3-dimercapto-, diethyl ester (9CI) (CA INDEX NAME)

publication year = 1997

L38 ANSWER 2 OF 15 HCA COPYRIGHT 2003 ACS 127:96339 Sulfur-containing (meth)acrylates for manufacture of scratch-resistant prastic lenses with high refractive index. Kobayashi, Seiichi; Kawauchi Keiya; Suzuki, Yoriyuki; Imai, Masao; Fujii, Kenichi (Mitsui Toatsu Chemicals, Inc., Japan). Jpn. Kokai Tokkyo Koho JP 09143153 (2 19970603 Helsei, 7 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1995-302729 19951121.

Compds. X[CO2(CH2):ISCOCR:CH2]m [R = H, Me; X = H2C:CRCOS(CH2)r, AB CH(SCOCR:CH2)CH2, CH(SCOCR:CH2)CH(SCOCR:CH2); m = 1, 2; n, r = 1-3] are prepd. and polymd. Thus, polymq. acryloylthioethyl acryloylthioacetate in the presence of tert-Bu peroxy-2-ethylhexanoate and 2-hydroxy-2-methyl-1phenylpropane-1-one in a mold gave a transparent lens with refractive index 1.591, Abbe no. 38.6, and good scratch resistance.

IC ICM C07C327-28

ICS C08F020-38; C08F220-38; G02B001-04; G02C007-02

38-3 (Plastics Fabrication and Uses) CC Section cross-reference(s): 23, 35, 73

38705-47-4P, 2-Mercaptoethyl thioglycolate 123097-82-5P ΙT 123173-76-2P 192130-47-5P 192130-48-6P 192130-49-7P RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(sulfur-contq. (meth) acrylate polymers for scratch-resistant lenses)

123097-82-5P 123173-76-2P TΤ

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(sulfur-contg. (meth)acrylate polymers for scratch-resistant lenses)

123097-82-5 HCA RN

Butanedioic acid, mercapto-, bis(2-mercaptoethyl) ester (9CI) (CA INDEX CN

RN 123173-76-2 HCA

Butanedioic acid, 2,3-dimercapto-, bis(2-mercaptoethyl) ester (9CI) (CA CN INDEX NAME)

L38 ANSWER 3 OF 15 HCA COPYRIGHT 2003 ACS

111:175367 Polythiols as resin improvers. Kanemura, Yoshinobu; Sasagawa, Katsuyoshi; Imai, Masao (Mitsui Toatsu Chemicals, Inc., Japan). Jpn. Kokai Tokkyo Koho JP 01090169 A2 19890406 Heisei, 3 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1987-244952 19870929.

HSCH2CH2OCOCHRCH(SH)CO2CH2CH2SH (R = H, SH) are useful in the manuf. of AΒ polythiourethanes having high refractive index and light dispersion characteristics. Thus, 25.22 g thiomalic acid was refluxed with 27.56 g 2-mercaptoethanol in C6H6 in the presence of p-MeC6H4SO3H to give 38.36 g thiomalic acid bis(2-mercaptoethyl ester) (I). Then, 18.1 g I was mixed with 18.8 g m-xylylene diisocyanate and 0.01 g dibutyltin laurate and heated in a mold at 80-120.degree. for 8 h to give a transparent and colorless resin with refractive index 1.62 and Abbe no. 35.

IC ICM C07C149-20

ICS C09K003-00

ICA C08G059-40; C08G065-34; C09K015-12; C10M135-26

ICI C10N030-10

CC 37-3 (Plastics Manufacture and Processing)

Section cross-reference(s): 23

IT 123097-82-5P, Thiomalic acid bis(2-mercaptoethyl ester)
 123173-76-2P, 2,3-Dimercaptosuccinic acid bis(2-mercaptoethyl ester)

RL: PREP (Preparation)

(prepn. and polymn. with diisocyanates)

1T 123097-82-5P, Thiomalic acid bis(2-mercaptoethyl ester)
123173-76-2P, 2,3-Dimercaptosuccinic acid bis(2-mercaptoethyl ester)

RL: PREP (Preparation)

(prepn. and polymn. with diisocyanates)

RN 123097-82-5 HCA

CN Butanedioic acid, mercapto-, bis(2-mercaptoethyl) ester (9CI) (CA INDEX NAME)

RN 123173-76-2 HCA

CN Butanedioic acid, 2,3-dimercapto-, bis(2-mercaptoethyl) ester (9CI) (CA INDEX NAME)

L38 ANSWER 4 OF 15 HCA COPYRIGHT 2003 ACS

102:96513 Heat stabilizers for halogenated resins. Bohen,
Joseph Michael; Reifenberg, Gerald Harvey (Pennwalt Corp., USA). Eur.
Pat. Appl. EP 124833 Al 19841114, 24 pp. DESIGNATED STATES: R:
BE, DE, FR, GB, NL. (English). CODEN: EPXXDW. APPLICATION: EP
1984-104741 19840427. PRIORITY: US 1983-489881 19830429.

AB Halogen-free heat stabilizer compns. for halogenated resins comprise (A) an aliph. mercaptan and (B) .gtoreq.1 S-contg. organotin compd., whereby .ltoreq.80% of the mercaptan can be replaced by an alkali or alk. earth metal salt of a mercaptan or mercapto acid and the A-B wt. ratio is (1-25):(1-20). Thus, PVC [9002-86-2] 100, paraffin wax 1.2, oxidized polyethylene wax 0.15, Ca stearate 0.6, CaCO3 2.0, TiO2 1.0, and 15:85 methyltin sesquisulfide + 2-mercaptoethyl stearate [27564-01-8] stabilizer 0.5 parts were mixed in a blender, masticated at 370.degree.F and rated visually for discoloration. A resin compn. contg. a binary stabilizer remained white after 15 min of processing, whereas a compn. contg. only 1 of the stabilizers was discolored after 3-12 min.

IC C08K005-37; C08K005-58; C08L027-06

CC 37-6 (Plastics Manufacture and Processing)

ST PVC heat stabilizer mercapto compd; tin mercaptide

```
heat stabilizer PVC; sulfide organotin heat
     stabilizer
IT
     Heat stabilizers
        (aliph. mercaptans and sulfur-contg. organotin compds., for halogenated
        resins)
ΙT
     Thiols, uses and miscellaneous
     RL: MOA (Modifier or additive use); USES (Uses)
        (aliph., heat stabilizers, contq. sulfur-contq.
        organotin compds., for halogenated resins)
TΤ
     Fatty acids, compounds
     RL: USES (Uses)
        (tallow, mercapto, tin salts, heat stabilizers, for
        halogen-contg. polymers)
IT
     9002-86-2
     RL: USES (Uses)
        (heat stabilizers for, aliph. mercaptans and
        sulfur-contg. organotin compds. as)
TΥ
     112-55-0 1185-81-5 4253-22-9 7440-31-5D, mercaptoethyltallow fatty
     acid salt, alkyl derivs. 7529-08-0 13269-74-4 22909-87-1
     25103-09-7
                  25168-24-5
                               25852-70-4
                                            26401-97-8
                                                         26636-01-1
     26761-46-6
                  27564-01-8
                               29946-28-9
                                            30374-01-7
                                                         30982-97-9
     54849-38-6
                  59118-76-2
                               59118-93-3
                                            59138-44-2
                                                         66368-81-8
     68298-40-8
                  69128-10-5
                               95115-32-5
                                            95115-33-6
                                                         95115-34-7
     95115-35-8
                95115-36-9
                               95115-37-0
                                            95115-38-1
     RL: MOA (Modifier or additive use); USES (Uses)
        (heat stabilizers, for halogenated resins)
IT
     7529-08-0
     RL: MOA (Modifier or additive use); USES (Uses)
        (heat stabilizers, for halogenated resins)
     7529-08-0 HCA
RN
     Butanedioic acid, mercapto-, dibutyl ester (9CI) (CA INDEX NAME)
CN
        SH
n-BuO-C-CH CH2-C-OBu-n
L38 ANSWER 5 OF 15 HCA COPYRIGHT 2003 ACS
101:212180 Stabilized poly(vinyl chloride) molding compositions. Upadek,
     Horst; Erwied, Werner; Wegemund, Bernd (Henkel K.-G.a.A., Fed. Rep. Ger.).
       Ger. Offen. DE 3247736 Al 19840705, 24 pp. (German). CODEN:
     GWXXBX. APPLICATION: DE 1982-3247736 19821223.
GI
```

AB Thiols I and RO2CCHRICHR2CO2R3 (R, R3, R4 = C5-22 alkyl; R1, R2 = H, SH) are useful as heat stabilizers for PVC [9002-86-2] molding compns. Thus, a mixt. of PVC 100, stearic acid 0.2, paraffin 0.2, pentaerythritol stearate 0.5, Zn stearate [557-05-1] 0.5, Ca stearate [1592-23-0] 1.0, zeolite NaA 1.0, and didecyl mercaptosuccinate [

```
58473-83-9] 0.5 part was processed at 170.degree. for 5 min and
    then heated at 180.degree.. The compn. was not discolored initially, was
    slightly discolored after 40 min, and was strongly discolored after 100
    C08L027-06; C08K005-10; C08K005-20; C08K005-37
IC
    37-6 (Plastics Manufacture and Processing)
CC
    PVC heat stabilizer mercaptosuccinic deriv; succinate
ST
    mercapto stabilizer PVC; succinimide mercapto alkyl stabilizer PVC;
    mercaptosuccinimide heat stabilizer PVC;
    mercaptosuccinate heat stabilizer PVC; thiol
    heat stabilizer PVC
ΙT
    Soaps
    Thiols, uses and miscellaneous
    RL: MOA (Modifier or additive use); USES (Uses)
        (heat stabilizers, for PVC)
ΙT
    Heat stabilizers
       (mercaptosuccinic derivs., for PVC)
    Zeolites, uses and miscellaneous
ΙT
    RL: MOA (Modifier or additive use); USES (Uses)
        (CaNaA, heat stabilizers, for PVC)
     Zeolites, uses and miscellaneous
TΤ
    RL: MOA (Modifier or additive use); USES (Uses)
       (NaA, heat stabilizers, for PVC)
ΙT
     9002-86-2
    RL: USES (Uses)
        (heat stabilizers for, mercaptosuccinic derivs. as)
     557-05-1 1592-23-0 6865-35-6 58473-83-9 93110-07-7
ΙT
     93110-08-8 93110-09-9
    RL: MOA (Modifier or additive use); USES (Uses)
        (heat stabilizers, for PVC)
TT
     58473-83-9 93110-07-7 93110-08-8
    RL: MOA (Modifier or additive use); USES (Uses)
        (heat stabilizers, for PVC)
     58473-83-9 HCA
RN
    Butanedioic acid, mercapto-, didecyl ester (9CI) (CA INDEX NAME)
CN
Me- (CH2) 9- O-C-CH2-CH-C-O- (CH2) 9-Me
RN
    93110-07-7 HCA
    Butanedioic acid, 2,3-dimercapto-, dihexyl ester (9CI) (CA INDEX NAME)
CN
Me- (CH2)5- O-C-CH-CH-C-O- (CH2)5-Me
RN
    93110-08-8 HCA
    Butanedioic acid, mercapto-, dioctadecyl ester (9CI) (CA INDEX NAME)
CN
                      SH O
Me^{-(CH_2)_{17}} O-C-CH<sub>2</sub>-CH-C-O-(CH<sub>2</sub>)<sub>17</sub>-Me
```

L38 ANSWER 6 OF 15 HCA COPYRIGHT 2003 ACS 101:212179 Stabilized poly(vinyl chloride) molding compositions. Upadek,

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Horst; Wegemund, Bernd; Erwied, Werner; Salz, Rainer (Henkel K.-G.a.A.,
      Fed. Rep. Ger.). Ger. Offen. DE 3247737 Al 19840705, 21 pp.
      (German). CODEN: GWXXBX. APPLICATION: DE 1982-3247737 19821223.
      Compds. RCOCH2SO3M (R = C1-18 alkyl, M = Na or K) are useful as
 AR
     heat stabilizers for PVC [9002-86-2] molding compns.
Thus, a mixt. of PVC 100, Ca stearate [1592-23-0] 1.0, Zn stearate
      [557-05-1] 0.5, stearic acid 0.2, paraffin 0.2, pentaerythritol stearate
      0.5, MeCOCH2SO3Na [16562-77-9] 0.5, and didecyl mercaptosuccinate
      58473-83-9] 0.5 part was processed at 170.degree. for 5 min and
      then heated at 180.degree.. The compn. was not discolored initially, was
      slightly discolored after 10 min, and was strongly discolored after 90
     min.
IC
     C08L027-06; C08K005-42
     37-6 (Plastics Manufacture and Processing)
CC
      PVC heat stabilizer oxoalkanesulfonate; sulfonate
     oxoalkane stabilizer PVC; calcium stearate stabilizer PVC; zinc stearate
     stabilizer PVC; stearate metal stabilizer PVC
ΙT
     Heat stabilizers
         (alkali metal oxoalkanesulfonates, for PVC)
IT
     Soaps
     RL: MOA (Modifier or additive use); USES (Uses)
         (heat stabilizers, for PVC)
IT
     Zeolites, uses and miscellaneous
     RL: MOA (Modifier or additive use); USES (Uses)
         (NaA, heat stabilizers, for PVC)
ΙT
     9002-86-2
     RL: USES (Uses)
         (heat stabilizers for, alkali metal
        oxoalkanesulfonates as)
IT
     557-05-1 1592-23-0 16562-77-9 19327-26-5 58446-52-9
     58473-83-9 78579-89-2
     RL: MOA (Modifier or additive use); USES (Uses)
         (heat stabilizers, for PVC)
ΙT
     58473-83-9
     RL: MOA (Modifier or additive use); USES (Uses)
         (heat stabilizers, for PVC)
RN
     58473-83-9 HCA
     Butanedioic acid, mercapto-, didecyl ester (9CI) (CA INDEX NAME)
CN
             O SH O
Me- (CH2) 9 O-C-CH2-CH-C-O- (CH2) 9-Me
L38 ANSWER 7 OF 15 HCA COPYRIGHT 2003 ACS
100:7895 Heat stabilizers for vinyl chloride polymers.
     Gay, Michel (Rhone-Poulenc Specialites Chimiques, Fr.). Eur. Pat. Appl. EP 90748 Al 19831005, 41 pp. DESIGNATED STATES: R: AT, BE, CH,
     DE, FR, GB, IT, LI, LU, NL, SE. (French). CODEN: EPXXDW. APPLICATION:
     EP 1983-420050 19830321. PRIORITY: FR 1982-5700 19820330.
     The title stabilizers, giving colorless transparent compns, contain org.
     compds. of Zn and of Group IIA metals and thiomalate diesters. Thus,
     plasticized PVC [9002-86-2] contg. Zn 2-ethylhexanoate [136-53-8] 0.09,
     Ba p-tert-butylbenzoate [10196-68-6] 0.5, and neopentyl glycol thiomalate
     (3:2) [88210-81-5] 0.80 phr when heated at 180.degree. had Gardner color
     O and 3 after 55 and 133 min, compared with 4 and black after 55 and 98
     min without the thiomalate.
IC
     C08L027-06; C08K005-00
CC
     37-6 (Plastics Manufacture and Processing)
```

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heat stabilizer PVC nonstaining; zinc carboxylate
     heat stabilizer; ethylhexanoate zinc heat
     stabilizer; barium carboxylate heat stabilizer
     ; butylbenzoate barium heat stabilizer; thiomalate
     ester heat stabilizer; neopentyl glycol thiomalate
     stabilizer
     Alkaline earth compounds
     RL: USES (Uses)
        (carboxylates, heat stabilizers, for PVC,
        nondiscoloring)
     Heat stabilizers
        (zinc-barium carboxylates and thiomalate esters, for PVC,
        nondiscoloring)
     136-53-8 557-04-0
ΙT
                         557-05-1 1592-23-0 4980-54-5 6865-35-6
     10196-68-6
                  52509-84-9 65291-46-5 77194-15-1 88210-81-5
     88210-82-6 88210-83-7 88228-75-5
     RL: MOA (Modifier or additive use); USES (Uses)
        (heat stabilizer, for PVC, nondiscoloring)
     9002-86-2
     RL: USES (Uses)
        (heat stabilizers for, metal carboxylates and
        thiomalate esters as nondiscoloring)
     RL: MOA (Modifier or additive use); USES (Uses)
        (heat stabilizer, for PVC, nondiscoloring)
     65291-46-5 HCA
CN
     Butanedioic acid, mercapto-, bis(2-ethylhexyl) ester (9CI) (CA INDEX
     NAME)
   Et-CH-Bu-n
L38 ANSWER 8 OF 15 HCA COPYRIGHT 2003 ACS
99:6547 Room temperature-crosslinking unsaturated polyester resins.
     Gallagher, Ronald B.; Novits, Michael F. (Pennwalt Corp., USA). U.S. US
     4380605 A 19830419, 7 pp. (English). CODEN: USXXAM.
    APPLICATION: US 1981-304136 19810921.
    Crosslinking of unsatd. polyesters at room temp. in the presence of a
    peroxyester initiator is accelerated by an org. mercapto compd. and a
    metal salt. Thus, 100 g Laminac 4123 [53529-34-3] polyester and 0.3 g
    mercaptobenzothiazole [149-30-4] were mixed, and 0.0003 g CuCl2 was added
     followed by 1.0 g tert-butylperoxybenzoate. Gel time was 16 min and cure
    time was 34 min. Without CuCl2, the gel time was 240 min, and with no
    accelerator it was 200 h.
    C08G063-76
NCL 525014000
    37-6 (Plastics Manufacture and Processing)
ΙT
    96-46-8 142-71-2 2935-90-2 4162-43-0 7529-08-0
    17356-08-0 30093-91-5 86100-20-1
    RL: CAT (Catalyst use); USES (Uses)
       (crosslinking catalyst contg., for unsatd. polyester)
ΤT
    7529-08-0
    RL: CAT (Catalyst use); USES (Uses)
       (crosslinking catalyst contg., for unsatd. polyester)
RN
    7529-08-0 HCA
```

04/07/2003

CN Butanedioic acid, mercapto-, dibutyl ester (9CI) (CA INDEX NAME)

L38 ANSWER 9 OF 15 HCA COPYRIGHT 2003 ACS
98:17449 New room-temperature cure system for RP. Kamath, V. R.; Novits, M. F.; Gallagher, R. B. (Lucidol Div., Pennwalt Corp., Buffalo, NY, USA).

Modern Plastics, 59(9), 90, 92, 94 (English) 1982. CODEN:

MOPLAY. ISSN: 0026-8275.

AB Initiator-promoter systems for crosslinking unsatd. polyesters are based on peroxyesters, promoted by mercaptan-metal salt mixts. The systems are adaptable to shelf life and cure times of com. processes, and they have good cost-performance data when compared to conventional cure systems.

CC 37-6 (Plastics Manufacture and Processing)
107-71-1 109-13-7 112-55-0 149-30-4 614-45-9 2372-21-6 2885-00-9 2935-90-2 3006-82-4 7447-39-4, uses and miscellaneous 7529-08-0 7705-08-0, uses and miscellaneous 13052-09-0 30093-91-5 RL: USES (Uses)

(catalyst compns. contg., for crosslinking polyesters)

IT 7529-08-0

RL: USES (Uses)

(catalyst compns. contg., for crosslinking polyesters)

RN 7529-08-0 HCA

CN Butanedioic acid, mercapto-, dibutyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|cccc} O & SH & O \\ \parallel & \parallel & \parallel \\ n-BuO-C-CH & CH_2-C-OBu-n \end{array}$$

L38 ANSWER 10 OF 15 HCA COPYRIGHT 2003 ACS 88:51589 Organotin mercapto dicarboxylic acid esters and compositions. Mack, Gerry P. (USA). U.S. US 4058543 19771115, 20 pp. (English). CODEN: USXXAM. APPLICATION: US 1976-646310 19760102.

AB The esters are useful for providing enhanced resistance to early and long-term discoloration in PVC [9002-86-2] resins, without imparting an obnoxious mercaptide odor to the compn. Thus, 2 mol aq. 10% NaOH was slowly added to a mixt. of 2 mol di-Bu thiomalate [7529-08-0] and 1 mol dimethyltin dichloride [753-73-1], and the soln. was heated 0.5 h at 60.degree. to give tetra-Bu [(dimethylstannylene)dithio]disuccinate (I). A mixt. of 1 mol I and 1 mol ethylene glycol was heated 3 h at 120-5.degree. to yield the dimethyltin thiomalate ester. Heating PVC contg. 2 phr ester 20 min. at 205.degree. resulted in a yellow color, compared to a light orange-brown color for similar resins contg. dimethyltin bis(isocctyl thioglycolate) or dimethyltin bis(di-Bu thiomalate) stabilizer. During milling, the controls emitted a strong mercapto ester odor, but no S odor was obsd. using the product ester.

NCL 260045750S

CC 36-6 (Plastics Manufacture and Processing) Section cross-reference(s): 29

ST PVC heat stabilizer; tin compd heat stabilizer; thiomalate tin deriv stabilizer

IT Heat stabilizers

04/07/2003

703-308-4139

```
(tin thiomalate derivs., for PVC)
ΙT
     9002-86-2
     RL: USES (Uses)
        (heat stabilizers for, tin thiomalate derivs. as)
TΤ
     65291-36-3D, reaction products with dioctyltin oxide
     RL: MOA (Modifier or additive use); USES (Uses)
        (heat stabilizers, for PVC)
TT
     105-08-8DP, esters with thiomalates 111-46-6DP, esters with thiomalates
     63979-81-7DP, reaction products with alkylene glycols
     65291-35-2P 65291-37-4P 65291-42-1P 65291-43-2DP,
     reaction products with alkylene glycols 65291-44-3DP, reaction products
     with alkylene glycols 65291-45-4DP, reaction products with
     alkylene glycols 65291-46-5DP, reaction products with alkylene
     glycols 65291-47-6DP, reaction products with alkylene glycols
     65291-48-7DP, reaction products with alkylene glycols
     RL: PREP (Preparation)
        (prepn. of)
ΙT
     7529-08-0
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with dialkyltin chlorides or oxides)
     1795-56-8
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with dimethyl [(dibutylstannyl)thio]succinate)
     65291-36-3D, reaction products with dioctyltin oxide
     RL: MOA (Modifier or additive use); USES (Uses)
        (heat stabilizers, for PVC)
RN
     65291-36-3 HCA
CN
     Butanedioic acid, mercapto-, 4-butyl 1-(2-hydroxyethyl) ester (9CI) (CA
     INDEX NAME)
HO-CH2-CH2 O-C-CH-CH2-C-OBu-n
     63979-81-7DP, reaction products with alkylene glycols
     65291-42-1P 65291-43-2DP, reaction products with
     alkylene glycols 65291-45-4DP, reaction products with alkylene
     glycols 65291-46-5DP, reaction products with alkylene glycols
     65291-47-6DP, reaction products with alkylene glycols
     RL: PREP (Preparation)
        (prepn. of)
     63979-81-7 HCA
RN
CN
     Butanedioic acid, mercapto-, didodecyl ester (9CI) (CA INDEX NAME)
Me- (CH2)11 O-C-CH2-CH-C-O- (CH2)11-Me
RN
     65291-42-1 HCA
     Butanedioic acid, mercapto-, 4,4'-(2,2-dimethyl-1,3-propanediyl)
CN
    1,1'-dibutyl ester (9CI) (CA INDEX NAME)
                          Me
n-BuO-C CH CH2-C-O-CH2-C-CH2-O-C-CH2-CH-C-OBu-n
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Page 14

John Calve, EIC - 1700, 308-4139

65291-43-2 HCA RN Butanedioic acid, mercapto-, bis(2-methylpropyl) ester (9CI) (CA INDEX CN

RN 65291-45-4 HCA

CN Butanedioic acid, mercapto-, dihexyl ester (9CI) (CA INDEX NAME)

65291-46-5 HCA RN

Butanedioic acid, mercapto-, bis(2-ethylhexyl) ester (9CI) (CA INDEX CN NAME)

Et-CH-Bu-n

RN 65291-47-6 HCA

Butanedioic acid, mercapto-, dipropyl ester (9CI) (CA INDEX NAME)

IT 7529-08-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with dialkyltin chlorides or oxides)

7529-08-0 HCA RN

Butanedioic acid, mercapto-, dibutyl ester (9CI) (CA INDEX NAME) CN

1795-56-8 ΙT

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with dimethyl [(dibutylstannyl)thio]succinate)

RN 1795-56-8 HCA

Butanedioic acid, mercapto-, dimethyl ester (9CI) (CA INDEX NAME)

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L38 ANSWER 11 OF 15 HCA COPYRIGHT 2003 ACS
86:56344 Hardening of epoxy resins. Senda, Hisakazu; Saeki, Shuji (Daiichi
Kogyo Seiyaku Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 51125499
      19761101 Showa, 3 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1975-50299 19750424.
AB
      Polyamines contg. di-Me tartarate (I) [608-68-4] or a similar compd. and
      optionally a polyamide were used as crosslinking agents to prep. epoxy
      resins having good weather- and water resistance. Thus, 100 parts Epikote
      828 [25068-38-6] was mixed with 8 parts diethylenetriamine [111-40-0] and
      3 parts I and hardened at 20.degree. for 2 h and 115.degree. for 30 min to
      prep. a resin having heat deformation temp. 115.degree., compared with
      95.degree. for a resin hardened in the absence of I.
     C08G059-58
CC
     36-6 (Plastics Manufacture and Processing)
      87-91-2 608-68-4 3333-46-8 17660-58-1
     RL: MOA (Modifier or additive use); USES (Uses)
         (crosslinking agents, contg. polyamines, for epoxy resins)
ΙT
     17660-58-1
     RL: MOA (Modifier or additive use); USES (Uses)
         (crosslinking agents, contg. polyamines, for epoxy resins)
RN
     17660-58-1 HCA
     Butanedioic acid, 2,3-dimercapto-, diethyl ester (9CI) (CA INDEX NAME)
CN
     O SH SH O
EtO-C-CH CH-C-OEt
L38 ANSWER 12 OF 15 HCA COPYRIGHT 2003 ACS
79:54841 Perfluoroalkyl group-containing mercaptans and sulfides. Falk,
     Robert A.; Kleiner, Eduard K. (Ciba-Geigy A.-G.). Ger. Offen. DE 2253051
     19730524, 71 pp. (German). CODEN: GWXXBX. APPLICATION: DE
     1972-2253051 19721028.
AΒ
     Reaction of a mercaptan contg. .geq.1 SH groups with a fluoroalkyl
     fumarate gave the title sulfides and reaction of thiomalonic acid
     [70-49-5] with 1,1,2,2-tetrahydroperfluorodecyl acetate [37858-04-1] gave
     bis(1,1,2,2-tetrahydroperfluorodecyl) mercaptosuccinate [
     41395-79-3]. The title compds. (24 used) were useful as oil and
     water repellents for cotton and Dacron fabrics. Thus, MeCCl3 contg.
     bis(1,1,2,2-tetrahydroperfluorodecyl) fumarate [33072-51-4], butanedithiol
     [1191-08-8], and Et3N was heated 24 hr at 60.deg. to give 75%
     tetrabis(1,1,2,2-tetrahydroperfluorodecyl) (tetramethylenedisthio)disuccin
     ate (I) [41395-81-7], m. 60-1.deg.. Dacron fabric treated with a 3% soln.
     of I (contg. 60.68\% F) in MeCCl3 exhibited an oil repellency rating of 6
     [on a scale of 1 (min.)-8(max.)] in AATCC test 118-1966T and a water
     repellency rating of 0 [on a scale of 0(min.)-100(max.)] in AATCC test
     22-1966 with 0.2% F on the fabric.
IC
     C07C; D06M
CC
     39-10 (Textiles)
     Section cross-reference(s): 23, 25
     39466-57-4 39466-58-5 41395-79-3
                                           41395-81-7
                                                      42941-36-6
     42941-37-7
                42941-38-8 42941-39-9
                                             42941-40-2
                                                          42941-41-3
                42941-43-5
     42941-42-4
                               43030-37-1
                                             43030-38-2
                                                          43193-00-6
     RL: USES (Uses)
        (soil repellents, for textiles)
IT
     41395-79-3
     RL: USES (Uses)
        (soil repellents, for textiles)
     41395-79-3 HCA
```

CN Butanedioic acid, mercapto-, bis(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl) ester (9CI) (CA INDEX NAME)

L38 ANSWER 13 OF 15 HCA COPYRIGHT 2003 ACS

79:54840 Free radical polymerization using perfluoroalkyl group-containing mercaptans as chain-transfer agents. Falk, Robert A.; Kleiner, Eduard (Ciba-Geigy A.-G.). Ger. Offen. DE 2253004 19730524, 74 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1972-2253004 19721028.

AB Polymers with low surface tension, esp. useful as antisoiling finishes for textiles, consisted of (RfACHR3CR1R2S)mB[S(M)q]nH or (RfACHR3CR1R2S)(M)qH, R1, R2, R3 = H, Me, RfA, RfACH2 with .geq.1 of R1, R2, R3 = RfA or RfACH2; Rf = perfluoroalkyl; A = a group of the type (CH2)kCO2, k = 0-10; B = combining atom or group, e.g., C; m = 0-10; n = 1-9; M = monomeric group; q = >1. The polymers were prepd. by polymg. the monomer in the presence of a perfluorogroup-contg. mercaptan chain-transfer agent, such as RfACHR3CR1R2SH. Thus, 10 parts 2:10 mercaptan chain-transfer agent [CBF17CH2CH2O2CH(SH)CH2CO2CH2CH2CBF17] [41395-79-3] - Me methacrylate (I) [80-62-6] mixt., 0.5% azobisisobutyronitrile (on wt. I) and 20 parts EtOAc were polymd. for 16 hr at 70.deg. to give a product contg. 0.85% F, no.-av. mol. wt. 6815, and crit. surface tension 14.3 dynes/cm compared with 39.0 dynes/cm for a sample similarly prepd. but using no mercaptan chain-transfer agent.

IC CO8F

CC 39-10 (Textiles)

L38 ANSWER 14 OF 15 HCA COPYRIGHT 2003 ACS

64:94282 Original Reference No. 64:17809f-h Stabilizing poly(vinyl halide) resins with a terpene and a sulfur-containing compound. Lindsey, William B. (E. I. du Pont de Nemours & Co.). US 3242133 19660322, 4 pp. (Unavailable). APPLICATION: US 19590708.

AB Poly(vinyl halides) can be heat stabilized by the use of a combination of an olefinically unsatd. terpene and 0 or a hydrocarbon or halogen deriv. of an olefinically unsatd. terpene and .gtoreq.1 compd. of the structure RSH or RSSR' in which R and R1 are alkyl, hydroxyalalkyl, thioalkyl, carboalkoxyalkyl, haloalkyl, arylalkyl, arylalkaryl, haloaryl, thioaryl, thioalkaryl, carboalkoxaryl, carboxyaryl, cycloalkyl, furyl, furfuryl, and thienyl groups. For example a mixt. of poly(vinyl chloride) resin 90, Lubridn V-3 2, beta.-pinene 5, and isooctyl thioglycolate 3 parts is extruded at 195.degree. through a conventional 1-in.-diam. extruder equipped with a 6-in. flat die and with a 0.007-in. opening and operating with a 50-100 mesh screen packs for 4 hrs. to produce a clear, essentially colorless, bubble-free film. In a control expt., a mixt. of 98 parts of the same poly(vinyl chloride) resin and 2 parts Lubiricin V-3 is fed into the same extruder at 195.degree.. It formed a bubble-contg. black mass in the heated zone of the extruder and plugged it.

NCL 45.7

CC 48 (Plastics Technology)

IT Gold chloride

(vinyl alc. polymer heat stabilization by

2-benzimidazolethiol and)

IT 7772-99-8, Tin chloride, SnCl2

(vinyl alc. polymer heat stabilization by

2-benzimidazolethiol and)

IT 91-60-1, 2-Naphthalenethiol 100-53-8, .alpha.-Toluenethiol 496-74-2,

Toluene-3,4-dithiol 1569-69-3, Cyclohexanethiol 2396-68-1, Benzenethiol, p-tert-butyl- 7072-70-0, Benzoic acid, o-mercapto-, butyl ester 7529-07-9, Propionic acid, 2-mercapto-, butyl ester 7529-08-0, Succinic acid, mercapto-, dibutyl ester 25103-09-7, Isooctyl alcohol, mercaptoacetate 25103-58-6, tert-Dodecyl mercaptan 28606-03-3, 2-Pinenethiol 30523-08-1, Propionic acid, 2-mercapto-, isooctyl ester

(vinyl halide resin stabilization by terpenes and)
IT 7529-08-0, Succinic acid, mercapto-, dibutyl ester
(vinyl halide resin stabilization by terpenes and)

RN 7529-08-0 HCA

CN Butanedioic acid, mercapto-, dibutyl ester (9CI) (CA INDEX NAME)

L38 ANSWER 15 OF 15 HCA COPYRIGHT 2003 ACS 58:33423 Original Reference No. 58:5693f-h,5694a-b Sulfur-containing dicarboxylic acids and derivatives. (F. Hoffmann-La Roche & Co., A.-G.). GB 9008986 19621024, 5 pp (Unavailable). PRIORITY: CH 19600226.

AB Racemic and optically active compds. were prepd. having the general formula [R'O2CCH(SR)]2, where R' is H or alkyl and R is H, alkyl or acyl, or RR is methylene. Thus, 380 g. HO2CC.tplbond.CCO2K was stirred over 0.5 hr., with cooling, into 500 ml. 5N HCl in EtOAc. After 1 hr., 380 g. AcSH was added dropwise over 2.5-3 hrs. at 35.degree., then stirred for 15 hrs. at 20 degree., and partitioned between H2O and EtOAc. The EtOAc soln. was concd. to 1 l. to ppt. 260 g. meso-2,3-bis(acetylthio) succinic acid. This was filtered off and recrystd. from EtOAc. The filtrate was concd., petr. ether added, and the ppt. boiled with Bu20 to give 75 g. dl-2,3-bis(acetylthio)succinic acid (I), m. 150-2.degree. (EtOAc-petr. ether), di-Me ester m. 70-1.degree.. I (19 g.) was dissolved in 190 ml. 3N NaOH, the soln. cooled to 0.degree., satd. with NaCl, made acid to Congo red with HCl, extd. with Et2O, and evapd. to yield 10.5 g. dl-2,3-dimercaptosuccinic acid (II), m. 126-7.degree. (iso-Pr2O), di-Me ester b0.01 80.degree. II (4.5 g.) was dissolved in 250 ml. MeOH and the soln. treated with 20 g. brucine dissolved in 250 ml. MeOH. The brucine salt of II (III) (23 g., m. 156-8.degree.) sepd. III was treated for 2 hrs. with N HCl and 9.4 q. solid (IV) was obtained as well as an acidic extract (V). IV was recrystd. once from MeOH and yielded a brucine salt, m. 275-80.degree.; the latter was dissolved in H2O, acidified with HCl, satd. with NaCl, extd. with Et2O, the Et2O evapd., and the residue recrystd. twice from EtOAc-petr. ether, to yield 100 mg. (+)-2,3-dimercaptosuccinic acid, m. 125-6.degree., [.alpha.]22D $128. \, \mathrm{degree}$. (c 1, Et20). V was satd. with NaCl, the soln. extd. 3 times with Et20 the Et20 evapd., and the residue recrystd. from C6H6, and then several times front EtOAc-petr. ether to yield (-)-2,3-dimercaptosuccinic acid, m. 125-6.degree., [.alpha.]22D -130.degree. (c 1, Et20). Similarly, I was treated with brucine in MeOH to give the salt, m. 130-1.degree., [.alpha.]21D -67.degree. (c 0.7, HCONMe2). The latter was hydrolyzed (NaOH) to give (-)-2,3-dimercaptosuccinic acid. Also prepd. were: d1-2,3-bis(acetylthio)succinic acid anhydride, m. 105-7.degree., (C6H6); di-Me dl-2,3-bis(methylthio)succinate, m. 72.degree. (iso-Pr20); 2,2-dimethyl-1,3-dithiolane-trans-4,5-dicarboxylic acid, m. 156-7.degree. (Et20-C6H6); 1,4-dithiaspiro[4,5]decane-trans-2,3-dicarboxylic acid, m. 184-5.degree. (Et20-petr. ether); 2-(p-chlorophenyl)-1,3-dithiolane-trans-4,5-dicarboxylic acid, m. 206-8.degree. (decompn.) (Et20-petr. ether).

These compds. were used as intermediates for the production of metal complexes for pharmaceuticals. They were also used directly as plant-protecting agents owing to their antifungal properties. They could be used as dusts (e.g., 1-10% in talc) and as sprays. 38 (Heterocyclic Compounds (More Than One Hetero Atom)) CC 17660-57-0, Succinic acid, 2,3-dimercapto-, dimethyl ester ΙT 37129-18-3, Succinic acid, 2,3-bis(methylthio)-, dimethyl ester 90927-64-3, Succinic acid, 2,3-dimercapto-, dimethyl ester, diacetate (prepn. of) ΙT 17660-57-0, Succinic acid, 2,3-dimercapto-, dimethyl ester (prepn. of) 17660-57-0 HCA RN Butanedioic acid, 2,3-dimercapto-, dimethyl ester (9CI) (CA INDEX NAME) CN

O SH SH O MeO-C-CH CH-C-OMe

=> d L39 1,10,20,30,40,50,60,70,80,90,100,110,120,130,140,150-155 cbib abs hitstr

L39 ANSWER 1 OF 155 HCA COPYRIGHT 2003 ACS

132:245323 Crystal structure of the nitridorhenium(V) derivative complex [ReN(CMe2PPhMe2)(DMSMe2)2]. Seifert, S.; Leibnitz, P.; Spies, H. (Bundesanstalt fur Materialforschung und -prufung, Berlin, Germany). Wissenschaftlich-Technische Berichte - Forschungszentrum Rossendorf, FZR-270, 154-155 (English) 1999. CODEN: WBFRFQ. ISSN: 1437-322X.

Reaction of ReNCl2(PMe2Ph)3 with 2,3-dimercaptosuccinic acid di-Me ester (DMSMe2) in Me Et ketone forms phosphoniomethylimido complex [ReN(CMe2PMe2Ph){DMSMe2}2] which was characterized by x-ray crystallog. A phosphine mol. is bound to the central C atom of the added solvent mol. and not, as expected, directly to the Re atom. The resulting Re:N-C-P chain has an angle N1-C13-P1 of 99.5.degree.. The Re-N bond length of 1.697 .ANG. is in the range of a double bonded N atom. A mechanism is proposed which involves reductive attack of a free phosphine mol. on a solvent mol. to form a carbonium ion and phosphine oxide. Addn. of the resulting electrophilic agent onto the nitrido atom and nucleophilic attack of a second phosphine results in product.

17660-57-0. Dimethyl 2,3-dimercaptosuccinate RL: RCT (Reactant); RACT (Reactant or reagent) (reaction with rhenium nitrido phosphine complex and Me Et ketone) RN • 17660-57-0 HCA

Butanedioic acid, 2,3-dimercapto-, dimethyl ester (9CI) (CA INDEX NAME)

MeO-C-CH CH-C-OMe

L39 ANSWER 10 OF 155 HCA COPYRIGHT 2003 ACS 127:315631 Arsenic-induced changes in certain neurotransmitter levels and their recoveries following chelation in rat whole brain. Tripathi, Neelima; Kannan, G. M.; Pant, B. P.; Jaiswal, D. K.; Malhotra, P. R.; Flora, S. J. S. (Division of Pharmacology and Toxicology, Defence Research and Development Establishment, Gwalior, 474002, India). Toxicology Letters, 92(3), 201-208 (English) 1997. CODEN: TOLED5. ISSN:

0378-4274. Publisher: Elsevier.

Arsenic as sodium arsenite (100 ppm in drinking water) was administered to AΒ male rats for 16 wk. Animals were then treated either with meso-2,3-dimercaptosuccinic acid (DMSA), sodium 2,3-dimercaptopropane 1-sulfonate (DMPS), di-Me DMSA (DmDMSA), or diisopropyl DMSA (DiPDMSA) twice daily (50 mg/kg) i.p. for 5 days. After 5 days of rest period, the animals were again given a second course of chelation therapy. The animals were sacrificed subsequently for the detn. of whole brain biogenic amines levels, acetylcholinesterase (AChE), monoamine oxidase (MAO) and .vdelta.~aminolevulinic acid dehydratase (ALAD) activities. A no. of biochem. parameters and arsenic concns. in some tissues were also detd. The results suggest a significant increase in brain arsenic concn. accompanied by alterations in neurotransmitters levels following As(III) exposure. Although chelation treatment was effective in reducing As burden, the altered biochem. variables responded less favorably to chelation therapy. The DMSA-diesters, particularly DiPDMSA, produced a more pronounced increase in brain arsenic burden, as well as alterations in a few neurotransmitters. It can be concluded that the lipophilic character of As antidotes may lead to unfavorable results following i.p. administration.

IT 27887-85-0, Dimethyl meso-2,3-dimercaptosuccinic acid 118311-05-0, Diisopropyl meso-2,3-dimercaptosuccinic acid RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(arsenic-induced changes in certain neurotransmitter levels and their recoveries following chelation in rat whole brain)

RN 27887-85-0 HCA

CN Butanedioic acid, 2,3-dimercapto-, dimethyl ester, (2R,3S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 118311-05-0 HCA

CN Butanedioic acid, 2,3-dimercapto-, bis(1-methylethyl) ester, (R^*,S^*) -(9CI) (CA INDEX NAME)

Relative stereochemistry.

L39 ANSWER 20 OF 155 HCA COPYRIGHT 2003 ACS

125:74600 Preparation, characterization, and enzymic hydrolysis of Re/Tc complexes with dimercaptocarboxylic acids and ethyl esters. Seifert, S.; Syhre, R.; Hoepping, A.; Klostermann, K.; Spies, H.; Johannsen, B. (Inst. Bioinorg. Radiopharm. Chem., Res. Cent. Rossendorf Inc., Dresden, D-01314,

Germany). Forschungszentrum Rossendorf e.V., [Bericht] FZR, FZR-122, 91-97 (English) 1996. CODEN: FRBFEU.

The influence of the no. and position of ester and free COOH groups in the ligands and the structure of ligand mols. on enzymic hydrolysis of square-pyramidal oxo complexes of Re(V) and Tc(V) with dithiolates was investigated. The ligands 2,3-dimercaptopropionic acid (DMPA), Et 2,3-dimercaptopropionate (DMPEt), and 1,1-dicarboethoxy-2,2-dithioethene (CETE) were studied. Complexes with these ligands and mixed complexes with these ligands and dimercaptosuccinic acid or its di-Et ester were prepd. and the hydrolysis behavior in solns. contg. pig liver esterase, rat plasma, or human plasma was studied in vitro and in vivo.

IT 17660-58-1, Dimercaptosuccinic acid diethyl ester

RL: RCT (Reactant); RACT (Reactant or reagent) (for prepn. technetium complexes with dimercaptocarboxylic acids and -carboxylates)

RN 17660-58-1 HCA

CN Butanedioic acid, 2,3-dimercapto-, diethyl ester (9CI) (CA INDEX NAME)

L39 ANSWER 30 OF 155 HCA COPYRIGHT 2003 ACS

123:46628 Different rates of enzymatic cleavage of the three stereoisomers of [ReO(DMS diester)2] - complexes. Seifert, S.; Syhre, R. (Germany). Forschungszent. Rossendorf, [Ber.] FZR, FZR-73, Institute of Bioinorganic and Radiopharmaceutical Chemistry, Annual Report, 1994, 42-5 (English) 1995. CODEN: FRBFEU.

AΒ [ReO(L)2]- (H2L = di-Me and di-Et and diisobutyl esters of meso-dimercaptosuccinic acid) were prepd. by the reaction of the diester with Bu4N[ReOCl4]. The reaction mixts, each contain mixts, of the three isomers (syn-exo, syn-endo, and anti) which were identified by proton NMR and, in the case of the di-Me and di-Et esters, sepd. by HPLC. The rates of enzymic hydrolysis by pig liver esterase were studied, and the syn-endo form was found to hydrolyze at a significantly faster rate than the other two isomers.

ΙT 27887-85-0, Dimethyl meso-2, 3-dimercaptosuccinate 101925-77-3 118908-62-6, Diisobutyl meso-2,3-

dimercaptosuccinate

RL: RCT (Reactant); RACT (Reactant or reagent)

(for prepn. of rhenium oxo dimercaptosuccinato diester complex stereoisomers)

RN 27887-85-0 HCA

CN Butanedioic acid, 2,3-dimercapto-, dimethyl ester, (2R,3S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 101925-77-3 HCA

Butanedioic acid, 2,3-dimercapto-, diethyl ester, (2R,3S)-rel- (9CI) (CA

INDEX NAME)

Relative stereochemistry.

RN 118908-62-6 HCA

CN Butanedioic acid, 2,3-dimercapto-, bis(2-methylpropyl) ester, (R*,S*)-(9CI) (CA INDEX NAME)

Relative stereochemistry.

L39 ANSWER 40 OF 155 HCA COPYRIGHT 2003 ACS
120:217089 Process for preparing beta-lactam derivatives (carbapenems) and azathiabicycloalkanes as synthetic intermediates thereof. Horikawa, Hiroshi; Kondo, Kazuhiko; Iwasaki, Tameo (Tanabe Seiyaku Co., Ltd., Japan). Eur. Pat. Appl. EP 559533 Al 19930908, 16 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE. (English). CODEN: EPXXDW. APPLICATION: EP 1993-400506 19930226. PRIORITY: JP 1992-99023 19920306.

AB .beta.-Lactams I [R1 = (un)protected hydroxyalkyl or amino; R2 = H, ester residue; X = CH2, alkylidene, S, ACH2; A = S, O, CH2; Y = OW, SR4; W = residue of active ester; R4 = org. group] and salts are prepd. by treating l-aza-3-thiabicycloalkanes II with a base and a desulfurizing agent, followed by reaction with an active esterifying agent and possibly with a mercaptan R4SH. Thus, (3S,4S)-3-[(R)-1-tert-butyldimethylsilyloxyethyl]-4-[(1R)-1-[2,2-bis(ethoxycarbonyl)ethylthiocarbonyl]ethyl]-1-[1-hydroxy-1-(pivaloyloxymethyloxycarbonyl)methyl]-2-azetidinone (prepn. given) was treated with SOCl2 and pyridine in THF at -40 to -50.degree. and the resultant 1-[1-chloro-1-(pivaloyloxymethyloxycarbonyl)methyl] deriv. was

cyclized by Et3N in DMF at -20 to 0.degree. to give (5R,6S,7R)-II [R1=(R)-Me3CSiMe2OCHMe, R2 = CH2OCOCMe3, X = .beta.-CHMe]. Desulfurization of this with KOCMe3 and PPh3 in PhMe at -40 to -20.degree. and esterification by quenching in a soln. of ClP(0) (OPh)2 in MeCN gave (1R,5S,6S)-I [R1=(R)-Me3CSiMe2OCHMe, R2 = CH2OCOCMe3, X = .beta.-CHMe] [III; Y=OP(0)] Treatment of this with (4S)-4-mercaptopyrrolidine-2-thione and (iso-Pr)2NEt in MeCN gave III [Y=(4R)-pyrrolidin-2-thion-4-ylthio]. A subset of I [i.e., R1=MeCH(OR6); R2 as given; X=CHMe; Y=1-R5-2-thioxopyrrolidinylthio; R5=H, alkyl, alkoxyalkyl, dialkylaminoalkyl; R6=H, protective group] are novel and show better antibacterial activity, stability to dehydropeptidase 1, oral absorbability, and toxicity in comparison to known analogs where Y is a 2-oxopyrrolidin-4-ylthio group.

IT 153492-39-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and thioesterification in prepn. of carbapenems)

RN 153492-39-8 HCA

CN Propanedioic acid, (mercaptomethyl)-, diethyl ester (9CI) (CA INDEX NAME)

0

L39 ANSWER 50 OF 155 HCA COPYRIGHT 2003 ACS

117:194853 A proposal of new prognostic criteria for lubricity of oils and nonoils lubricating liquids. Tokarzewski, L.; Borek, J. (Inst. Chem., Silesian Univ., Katowice, Pol.). Rivista Italiana delle Sostanze Grasse, 69(4), 219 (English) 1992. CODEN: RISGAD. ISSN: 0035-6808.

AB A combination of high mol. polarizability and small wetting angles predicts the lubricity (welding load) of lubricants, base oils, and individual compds., e.g., xylene, PhNO2, ethylene glycol, etc.

IT 65291-46-5 RL: USES (Uses)

(lubricity of, prediction of, polarizability and wetting angle in)

RN 65291-46-5 HCA

CN Butanedioic acid, mercapto-, bis(2-ethylhexyl) ester (9CI) (CA INDEX NAME)

L39 ANSWER 60 OF 155 HCA COPYRIGHT 2003 ACS

114:116515 The mobilization of intracellular cadmium by alkoxyethyl esters of
 meso-2,3-dimercaptosuccinic acid. Jones, Mark M.; Singh, Pramod K.; Gale,
 Glen R.; Atkins, Loretta M.; Smith, Alayne B. (Cent. Mol. Toxicol.,
 Vanderbilt Univ., Nashville, TN, 37235, USA). Toxicology and Applied
 Pharmacology, 106(3), 529-35 (English) 1990. CODEN: TXAPA9.
 ISSN: 0041-008X.

AB The Cd-mobilizing properties of 2 newly synthesized esters of meso-2,3-dimercaptosuccinic acid in mice have been examd. They are bis(2'-methoxyethyl) meso-2,3-dimercaptosuccinate (MEDMS) and

bis(2'-ethoxyethyl) meso-2,3-dimercaptosuccinate (EEDMS), conveniently prepd. from dimercaptosuccinic acid with 2-methoxyethanol and 2-ethoxyethanol, resp. Mobilization studies in mice of aged in vivo Cd deposits using 5 i.p. injections of 0.40 mmol/kg of each chelator in peanut oil clearly indicate that MEDMS and EEDMS are significantly superior to BAL in depleting the whole body burden of Cd. The redns. caused by MEDMS and EEDMS were .apprx.20% and 26%, resp., whereas under similar dosage regimens BAL effected about only a 12% redn. The esters were neither equal nor superior to BAL for the redn. of renal Cd levels, MEDMS being the least effective. For the mobilization of hepatic Cd deposits, both were quite promising (MEDMS, 20%; EEDMS, 34% redn.) compared to BAL (only 2% redn.). There was no accumulation of Cd with either MEDMS or EEDMS in any of the other organs examd.: spleen, testes, pancreas, and particularly the brain. These compds. enhance the fecal excretion of Cd by a factor of 25-40-fold, but have very little effect on the urinary excretion of this element. Thus, the order of overall efficacy is EEDMS > MEDMS > BAL, considering the liver and whole body burdens of Cd, but BAL > EEDMS > MEDMS in terms of the efficacy in reducing Cd levels in the kidneys.

IT 132572-49-7P 132572-50-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of and cadmium mobilization by)

RN 132572-49-7 HCA

CN Butanedioic acid, 2,3-dimercapto-, bis(2-methoxyethyl) ester, (R*,S*)-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 132572-50-0 HCA

CN Butanedioic acid, 2,3-dimercapto-, bis(2-ethoxyethyl) ester, (R^*,S^*) -(9CI) (CA INDEX NAME)

Relative stereochemistry.

L39 ANSWER 70 OF 155 HCA COPYRIGHT 2003 ACS

111:52417 The role of non-specific esterases in insecticide resistance to malathion in the diamondback moth Plutella xylostella. Doichuanngam, K.; Thornhill, R. A. (Dep. Zool. Comp. Physiol., Univ. Birmingham, Birmingham, B15 2TT, UK). Comparative Biochemistry and Physiology, Part C: Pharmacology, Toxicology & Endocrinology, 93C(1), 81-5 (English) 1989. CODEN: CBPCEE. ISSN: 0742-8413.

AB Esterases play an important role in the mechanism of resistance to malathion in the diamondback moth P. xylostella. These enzymes metabolize

malathion to less toxic metabolites such as malathion monocarboxylic acid and malathion dicarboxylic acid. The rate of metab. to nontoxic compds. is more rapid in the resistant strain compared with the susceptible strain. Selection of the susceptible strain with malathion over 8 generations gives rise to an increased resistance to malathion that can be correlated with an increase in esterases, particularly in carboxylesterases.

IT 23060-14-2

RL: BIOL (Biological study)

(malathion metabolite in diamondback moth, detoxication in relation to)

RN 23060-14-2 HCA

CN Butanedioic acid, mercapto-, diethyl ester (9CI) (CA INDEX NAME)

L39 ANSWER 80 OF 155 HCA COPYRIGHT 2003 ACS 109:22910 Thio ketones and enethiolates by 1,3-anionic cycloreversion of dithiolane derivatives. Schaumann, Ernst; Ruehter, Gerd (Inst. Org. Chem., Univ. Hamburg, Hamburg, D-2000/13, Fed. Rep. Ger.). Chemische Berichte, 121(6), 1159-63 (German) 1988. CODEN: CHBEAM. ISSN: 0009-2940. OTHER SOURCES: CASREACT 109:22910.

GI

AB The reactive thioketones, RR1C:S [R = R1 = Me; RR1 = (CH2)5; R = Me, R1 = Ph] were generated by cycloreversion of the anions of 1,3-dithiolane-4,5-dicarboxylates I and were trapped by mesitonitrile oxide in a 1,3-dipolar cycloaddn. to give oxathiazoles II. From the fragmentation of anions of 1,3-dithiolane 1,1-dioxides III (R = R1 = Me, Ph; R = Me, R1 = Ph), thiobenzophenone was isolated, whereas thioketones RR1C:S (R = R1 = Me; R = Me, R1 = Ph) with an .alpha.-hydrogen were deprotonated in situ to provide enethiolates CH2:CR1S- which on treatment with 2,4,6-Me3C6H2C.tplbond.NO gave thiohydroximates 2,4,6-Me3C6H2C(:NOH)SC(:CH2)R1.

IT 27887-85-0

RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclocondensation of, with ketones)

RN 27887-85-0 HCA

CN Butanedioic acid, 2,3-dimercapto-, dimethyl ester, (2R,3S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L39 ANSWER 90 OF 155 HCA COPYRIGHT 2003 ACS
105:78477 Fragmentation of 1,3-dithiolane-derived sulfur ylides. A convenient thioaldehyde synthesis. Schaumann, Ernst; Ruehter, Gerd (Inst. Org. Chem., Univ. Hamburg, Hamburg, D-2000/13, Fed. Rep. Ger.). Tetrahedron Letters, 26(43), 5265-8 (English) 1985. CODEN: TELEAY. ISSN:

GT

$$R^{1}$$
 S R^{2} S R^{2}

AB Thioacetalization of R1CHO (R1 = H, Me, Me3C, Ph, CH2:CH) with R2CH(SH)CH(SH)R2 (R2 = CO2H, CO2Me, Ph) gave the dithiolanes I. I were methylated, then regiospecifically deprotonated to give the thioaldehydes R1CHS, which were trapped with mesitonitrile oxide.

IT 27887-85-0

RL: RCT (Reactant); RACT (Reactant or reagent)

0040-4039. OTHER SOURCES: CASREACT 105:78477.

(reaction of, with aldehydes)

RN 27887-85-0 HCA

CN Butanedioic acid, 2,3-dimercapto-, dimethyl ester, (2R,3S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L39 ANSWER 100 OF 155 HCA COPYRIGHT 2003 ACS

- 99:135485 Formation of metabolites of malathion during storage of wettable powder formulations. Roy, Pranab; Sarup, Prakash (Div. Entomol., Indian Agric. Res. Inst., New Delhi, 110012, India). Journal of Entomological Research, 5(2), 183-7 (English) 1981. CODEN: JEREDP. ISSN: 0378-9519.
- AB Various malathion [121-75-5] wettable powder formulations were subjected to long-term storage at ambient temp. and to accelerated storage under uniform pressure of 25 g/cm2 at 54.degree. for 24 h. The bioefficacy of such formulations was evaluated against the adults of Sitophilus oryzae. The most effective formulation involved diluents bentonite + diatomite and Lissapol D [8063-52-3] as wetting agent, or deactivated fuller's earth

and Hyoxyd AAO [78810-06-7] as wetting agent. The least effective formulation was based on China clay + fuller's earth as diluents, irresp. of these wetting agents. Two metabolites of malathion formed during storage of formulations differed in their concns. TLC suggested that ester groups might not have suffered any degrdn., but cleavage occurred at the P-S bond.

TΤ 23060-14-2

> RL: BIOL (Biological study) (malathion degrdn. product, formation during storage of wettable powder formulations)

23060-14-2 HCA RN

CN Butanedioic acid, mercapto-, diethyl ester (9CI) (CA INDEX NAME)

L39 ANSWER 110 OF 155 HCA COPYRIGHT 2003 ACS

93:102019 Kinetic investigations on the reaction of technetium(V) gluconate with meso-dimercaptosuccinic acid and meso-dimercaptosuccinic acid dimethylester. Spies, H.; Johannsen, B.; Muenze, R.; Unverferth, K. (Cent. Inst. Nucl. Res., Rossendorf, Ger. Dem. Rep.). Radiochemical and Radioanalytical Letters, 43(5), 311-18 (English) 1980. CODEN: RRALAZ. ISSN: 0079-9483.

AB Results concerning the kinetics of the ligand exchange reaction of Tc(V) gluconate with mesodimercaptosuccinic acid and meso-dimercaptosuccinic acid dimethyl ester, resp., are presented.

IT 27887-85-0

> RL: RCT (Reactant); RACT (Reactant or reagent) (substitution reaction of, for gluconate in technetium(V) complex, kinetics of)

RN 27887-85-0 HCA

Butanedioic acid, 2,3-dimercapto-, dimethyl ester, (2R,3S)-rel- (9CI) (CA CN INDEX NAME)

Relative stereochemistry.

L39 ANSWER 120 OF 155 HCA COPYRIGHT 2003 ACS 87:84943 Synthesis of thiopyrano[2,3-d]pyrimidines and thieno[2,3d]pyrimidines. Santilli, Arthur A.; Scotese, Anthony C. (Res. Dev. Div., Wyeth Lab., Inc., Radnor, PA, USA). Journal of Heterocyclic Chemistry, 14(3), 361-5 (English) 1977. CODEN: JHTCAD. ISSN: 0022-152X. GΙ

AB The reaction of 4-chloro-5-cyano-2-methylthiopyrimidine with EtO2CCH2CH(SH)CO2Et in refluxing EtOH gave diethyl 5-amino-2-(methylthio)-7H-thiopyrano[2,3-d]pyrimidine-6,7-dicarboxylate (I). Displacement of the methylthio group in I with H2NNH2 gave the corresponding hydrazino deriv. which underwent Schiff base formation with PhCHO or 2,6-C12C6H3CHO. Treatment of I in Ac20 gave the corresponding diacetylated amino deriv. Partial sapon. of I with NaOH gave 5-amino-2-(methylthio)-7Hthiopyrano[2,3-d]pyrimidine-6,7-dicarboxylic acid 6 ethyl ester. reaction of 4-amino-6-chloro-5-cyano-2-phenylpyrimidine with EtO2CCH2CH(SH)CO2Et resulted in the formation of Et 4-amino-6-(ethoxycarbonyl)-5,6-dihydro-5-amino-2-phenylthieno[2,3-d]pyrimidine-6acetate (III), which when subjected to hydrolysis, gave Et 4,5-diamino-2-phenylthieno[2,3-d]pyrimidine-6-acetate-HCl. Diazotization of I with NaNO2 in HOAc gave diethyl 5-(acetyloxy)-6,7-dihydro-6-hydroxy-2-(methylthio)-5H-thiopyrano[2,3-d]pyrimidine-6,7-dicarboxylate (IV). ΙT 23060-14-2

RL: RCT (Reactant); RACT (Reactant or reagent) (cyclization of, with chloro(methylthio)cyanopyrimidine, thiopyranopyrimidinedicarboxylate deriv. from) 23060-14-2 HCA

RN

Butanedioic acid, mercapto-, diethyl ester (9CI) (CA INDEX NAME) CN

L39 ANSWER 130 OF 155 HCA COPYRIGHT 2003 ACS

78:110476 Influence of substituents on preparation and tautomerism of open-chain .beta.-thio keto esters. Structure determination by NMR and infrared spectroscopy. Duus, F. (Dep. Chem., Aarhus Univ., Aarhus, Den.). Tetrahedron, 28(24), 5923-47 (English) 1972. CODEN: TETRAB. ISSN: 0040-4020.

GI For diagram(s), see printed CA Issue.

AΒ The acid-catalyzed reactions of 36 .beta.-keto esters, RCOCHR1CO2R2 (I), with H2S were studied. Passing H2S and HCl at -60.degree. or higher temps. through I (R1 = H) in MeCN or EtOH gave tautomers of RCSCHR1CO2R2 (II), whereas .alpha.-substituted I gave gem-dithiols, RC(SH)2CHR1CO2R2, or II depending on R1 and the reaction conditions. Alkyl halides and II Ti(I) salts gave S-alkylation. NMR and ir showed that the .beta.-thioxo esters II (R1 = H) exist as the intramol. H-bonded cis-enethiol tautomers (III). The .alpha.-substituted esters exist as approx. 1:1 mixts. of the

cis- and trans-enethiols, due to steric crowding. NMR chem. shifts as indicators of intramol. H-bonding and the long-range through-bond and through-space couplings involving enethiclic protons were discussed.

ΙT 20621-66-3P 40553-26-2P 40553-33-1P

40553-51-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 20621-66-3 HCA

CN Propanedioic acid, (1-mercaptoethylidene)-, diethyl ester (9CI) (CA INDEX NAME)

RN 40553-26-2 HCA

2-Pentenedioic acid, 3-mercapto-, diethyl ester (9CI) (CA INDEX NAME) CN

RN 40553-33-1 HCA

Pentanedioic acid, 2-(1-mercaptoethylidene)-, diethyl ester, (Z)- (9CI) CN (CA INDEX NAME)

Double bond geometry as shown.

RN 40553-51-3 HCA

CN Pentanedioic acid, 2-(1-mercaptoethylidene)-, diethyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L39 ANSWER 140 OF 155 HCA COPYRIGHT 2003 ACS

RN

63:54225 Original Reference No. 63:9821c-d Preparation of butyl ester of methylenebis(thioglycolic acid). Haase, Hans J.; Grimm, Horst DD 31323 19650501, 2 pp. (Unavailable). APPLICATION: DD 19620831.

AB Crude methylenebis(thioglycolic acid) was esterified directly with BuOH in the absence of mineral acid catalyst. A mixt. of 175 kg. 90% thioglycolic acid and 71 kg. 36.5% aq. HCHO was warmed to 70.degree. to initiate an exothermic reaction that brought the mixt. to boiling, 45 l. H2O distd., 210 kg. BuOH added, heating continued 10 hrs. while removing water azeotropically, and excess BuOH removed by warming to b60-70 135.degree. to recover 264 kg. title compd. as a yellow oil.

IT 3659-03-8, Glutaric acid, 2,4-dimercapto, dibutyl ester

(prepn. of) 3659-03-8 HCA

CN Glutaric acid, 2,4-dimercapto-, dibutyl ester (7CI, 8CI) (CA INDEX NAME)

L39 ANSWER 150 OF 155 HCA COPYRIGHT 2003 ACS
54:67782 Original Reference No. 54:12973e-i,12974a Incorporation of
 mercaptomethyl groups into .beta.-dicarbonyl compounds by means of
 chloromethyl acetyl sulfide. Bohme, H.; Kreitz, K.; Nurnberg, E. (Univ.
 Marburg, Germany). Arch. Pharm., 292, 456-61 (Unavailable) 1959

cf. CA 49, 2322f. EtCO2CHMeCO2Et (I), AcCHMeCO2Et (II), or AB .alpha.-methylindandione (III) reacted as their Na compds. with ClCH2SAc (IV) (CA 54, 10931a). Thus, 17.4 g. I was added dropwise to 2.3 g. Na in 120 ml. Et2O (after the Na had dissolved), 12.5 g. IV in 40 ml. Et2O added, the mixt. stirred until colorless, heated on a water bath 30 min., ice-cold H2O added, the Et2O phase sepd., extn. with Et2O twice repeated, the combined Et2O exts. concd., and fractionated to give 14.1 g. EtCO2CMe(CH2SAc)CO2Et, bl1 160.degree., which (26.2 g.) dissolved in 200 ml. N HCl-abs. EtOH and kept 60 hrs. at room temp. gave on fractionation 19.8 g. EtCO2CMe(CH2SH)CO2Et (V), b10 125.degree.. Oxidn. of 2.2 g. V with N iodine-MeOH gave 3.5 g. bis(.beta.,.beta.'-dicarbethoxypropyl) disulfide, bl0-2 100-20.degree.). With 14.4 g. II instead of I the same reactions yielded 13 g. AcCMe(CH2SAc)CO2Et (VI), b12 143.degree., which (11.7 g.) on addn. of 105 ml. 1.5N HCl-abs. EtOH gave 5.7 g. AccMe(CH2SH)CO2Et, b12 126.degree., which (5.7 g.) was converted like V to 5 g. bis(.beta.-acetyl-.beta.-carbethoxypropyl) disulfide, b0.05 130-40.degree.. By the same reactions, 37.5 g. Et 2-(acetylthiomethyl)-1cyclohexanone-2-carboxylate (VII), b0.05 122.degree., was prepd. from 57 g. Et cyclohexanone-2-carboxylate, 7.7 g. Na, and 41.3 g. IV, with C6H6 instead of Et20 as solvent. VII (20 g.) was converted like VI to 8 g. Et 2-mercaptomethyl-1-cyclohexanone-2-carboxylate, b0.01 86-8.degree., n24.5D 1.4920. This (6.5 g.) was treated like V to give 3 g. bis(1-cyclohexanone-2-carboxylic acid ethyl ester) 2,2'-methylene disulfide, b0.001 165.degree., n23D 1.5145. Et 2-(acetylthiomethyl)-1cyclopentanone-2-carboxylate (21 g.), b0.1 122.degree., was prepd. like VII with 68 g. K salt of Et cyclopentanone-2-carboxylate. With 9.1 g. Na deriv. of III instead of Na deriv. of I and 0.2 g. IV with MeOH solvent, and addn. of H2O and Et2O after heating, the Et2O ext. obtained yielded on standing 10 g. .alpha.-methyl-.alpha.-acetylthiomethylindandione, m. 93.degree. (MeOH), which (12.4 g.), treated with HCl, yielded on fractionation 9 g. .alpha.-methyl-.alpha.-mercaptomethylindandione, b0.01 60.degree., m. 47.5.degree., which (10.3 g.), oxidized with KI-H2O2, yielded 9 g. .alpha.-methylbisindandionylmethyl) disulfide, m. 119.degree.

- 63:54225 Original Reference No. 63:9821c-d Preparation of butyl ester of methylenebis(thioglycolic acid). Haase, Hans J.; Grimm, Horst DD 31323 19650501, 2 pp. (Unavailable). APPLICATION: DD 19620831.
- AB Crude methylenebis(thioglycolic acid) was esterified directly with BuOH in the absence of mineral acid catalyst. A mixt. of 175 kg. 90% thioglycolic acid and 71 kg. 36.5% aq. HCHO was warmed to 70.degree. to initiate an exothermic reaction that brought the mixt. to boiling, 45 l. H2O distd., 210 kg. BuOH added, heating continued 10 hrs. while removing water azeotropically, and excess BuOH removed by warming to b60-70 135.degree. to recover 264 kg. title compd. as a yellow oil.
- RN 3659-03-8 HCA
- CN Glutaric acid, 2,4-dimercapto-, dibutyl ester (7CI, 8CI) (CA INDEX NAME)

- L39 ANSWER 150 OF 155 HCA COPYRIGHT 2003 ACS 54:67782 Original Reference No. 54:12973e-i,12974a Incorporation of mercaptomethyl groups into .beta.-dicarbonyl compounds by means of chloromethyl acetyl sulfide. Bohme, H.; Kreitz, K.; Nurnberg, E. (Univ. Marburg, Germany). Arch. Pharm., 292, 456-61 (Unavailable) 1959
- AB cf. CA 49, 2322f. EtCO2CHMeCO2Et (I), AcCHMeCO2Et (II), or .alpha.-methylindandione (III) reacted as their Na compds. with ClCH2SAc (IV) (CA 54, 10931a). Thus, 17.4 g. I was added dropwise to 2.3 g. Na in 120 ml. Et20 (after the Na had dissolved), 12.5 g. IV in 40 ml. Et20 added, the mixt. stirred until colorless, heated on a water bath 30 min., ice-cold H2O added, the Et2O phase sepd., extn. with Et2O twice repeated, the combined Et20 exts. concd., and fractionated to give 14.1 g. EtCO2CMe(CH2SAc)CO2Et, b11 160.degree., which (26.2 g.) dissolved in 200 ml. N HCl-abs. EtOH and kept 60 hrs. at room temp. gave on fractionation 19.8 g. EtCO2CMe(CH2SH)CO2Et (V), bl0 125.degree.. Oxidn. of 2.2 g. V with N iodine-MeOH gave 3.5 g. bis(.beta.,.beta.'-dicarbethoxypropyl) disulfide, b10-2 100-20.degree.). With 14.4 g. II instead of I the same reactions yielded 13 g. AcCMe(CH2SAc)CO2Et (VI), b12 143.degree., which (11.7 g.) on addn. of 105 ml. 1.5N HCl-abs. EtOH gave 5.7 g. AcCMe(CH2SH)CO2Et, b12 126.degree., which (5.7 g.) was converted like V to 5 g. bis(.beta.-acetyl-.beta.-carbethoxypropyl) disulfide, b0.05 130-40.degree. By the same reactions, 37.5 g. Et 2-(acetylthiomethyl)-1cyclohexanone-2-carboxylate (VII), b0.05 122.degree., was prepd. from 57 g. Et cyclohexanone-2-carboxylate, 7.7 g. Na, and 41.3 g. IV, with C6H6 instead of Et2O as solvent. VII (20 g.) was converted like VI to 8 g. Et 2-mercaptomethyl-1-cyclohexanone-2-carboxylate, b0.01 86-8.degree., n24.5D 1.4920. This (6.5 g.) was treated like V to give 3 g. bis(1-cyclohexanone-2-carboxylic acid ethyl ester) 2,2'-methylene disulfide, b0.001 165.degree., n23D 1.5145. Et 2-(acetylthiomethyl)-1cyclopentanone-2-carboxylate (21 g.), b0.1 122.degree., was prepd. like VII with 68 g. K salt of Et cyclopentanone-2-carboxylate. With 9.1 g. Na deriv. of III instead of Na deriv. of I and 0.2 g. IV with MeOH solvent, and addn. of H2O and Et2O after heating, the Et2O ext. obtained yielded on standing 10 g. .alpha.-methyl-.alpha.-acetylthiomethylindandione, m. 93.degree. (MeOH), which (12.4 g.), treated with HCl, yielded on fractionation 9 g. .alpha.-methyl-.alpha.-mercaptomethylindandione, b0.01 60.degree., m. 47.5.degree., which (10.3 g.), oxidized with KI-H2O2, yielded 9 g. .alpha.-methylbisindandionylmethyl) disulfide, m. 119.degree.

(MeOH-H2O). Instead of IV, AcOCH2Cl (VIII) could be used for incorporation of the acetoxymethyl group by analogous reactions. Thus, 55 g. K salt of Et cyclopentanone-2-carboxylate in 250 ml. abs. C6H6 was stirred with 31.2 g. VIII, refluxed, filtered from the KCl, concd. in vacuo, and fractionated to give 23 g. Et 2-acetoxymethyl-1-cyclopentanone-2-carboxylate, b0.05 90-3.degree.. Similarly, 50 g. Me cyclopentanone-2-carboxylate and 30.5 g. VIII yielded 13 g. Me 2-acetoxymethyl-1-cyclopentanone-2-carboxylate, b9 150-4.degree..

- ΙT 99183-68-3, Malonic acid, (mercaptomethyl) methyl-, diethyl ester (prepn. of)
- 99183-68-3 HCA RN
- CN Malonic acid, (mercaptomethyl)methyl-, diethyl ester (6CI) (CA INDEX NAME)

- L39 ANSWER 151 OF 155 HCA COPYRIGHT 2003 ACS
- 53:114399 Original Reference No. 53:20529e-f Skin sensitization by mercaptans of low molecular weight. Voss, J. G. (Procter & Gamble Co., Cincinnati, O.). J. Invest. Dermatol., 31, 373-9 (Unavailable) 1958.
- Mercaptans in concns. equiv. to 1.25% thioglycolate were applied in patch AB tests, left in situ for 24 hrs., and repeated 3 times weekly for 3 weeks. After 10 days fresh patches were applied to the original sites and to fresh sites adjacent to the original site to distinguish between hypersensitivity and skin fatigue. Of 44 compds. tested 40 were found to sensitize man and (or) guinea pig. Thioglycolic and 3-mercaptopropionic acid showed no allergenic activity; derivs. of thioglycolamide were usually the most strongly allergenic. Cross-sensitization to thioglycolate by other mercaptans was observed in 3 cases.
- 91007-96-4, Succinic acid, mercapto-, bis(2-methoxyethyl) ester (skin sensitization by)
- RN 91007-96-4 HCA
- Succinic acid, mercapto-, bis(2-methoxyethyl) ester (6CI, 7CI) (CA INDEX CN

- L39 ANSWER 152 OF 155 HCA COPYRIGHT 2003 ACS
- 51:66416 Original Reference No. 51:11999d Decomposition of diazo ketones by cuprous oxide. III. Synthesis of hexatetracontane-1,46-dioic acid. Hnevsova, Vera; Smely, Vaclav; Ernest, Ivan Collection Czech. Chem. Communs., 21, 1459-66 (German) 1956. See C.A. 50, 13749b. 23060-14-2, Succinic acid, mercapto-, diethyl ester
- AB
- IΤ (prepn. of)
- RN 23060-14-2 HCA
- Butanedioic acid, mercapto-, diethyl ester (9CI) (CA INDEX NAME) CN

- L39 ANSWER 153 OF 155 HCA COPYRIGHT 2003 ACS
- 51:66415 Original Reference No. 51:11999d Preparing mercaptosuccinic acid. Emr, Antonin; Roubinek, Frantisek Collection Czech. Chem. Communs., 21, 1651-3 (German) 1956.
- AB See C.A. 50, 8460d.
- 23060-14-2, Succinic acid, mercapto-, diethyl ester TT
- (prepn. of)
- 23060-14-2 HCA
- CN Butanedioic acid, mercapto-, diethyl ester (9CI) (CA INDEX NAME)

- L39 ANSWER 154 OF 155 HCA COPYRIGHT 2003 ACS
- 51:47164 Original Reference No. 51:8782g-h Preparing thiomalic acid and its ethyl ester. Emr, Antonin CS 85677 19560615 (Unavailable). APPLICATION: CS .
- Into 1200 ml. dry pyridine (I) satd. at -10.degree. with dry H2S to AB contain 55-60 mg. H2S/ml. is dropped with stirring and bubbling of H2S 120 g. di-Et fumarate in 120 ml. dry I at 5-10.degree.. After stirring at room temp. for 1-1.5 hrs. under continuous bubbling of H2S, I is distd. in vacuo and the residue distd. to give 115 g. di-Et thiomalate, b9 120.degree.. The main side product is di-Et thiodisuccinate, b0.1 154.degree..
- 23060-14-2, Succinic acid, mercapto-, diethyl ester (prepn. of)
- RN 23060-14-2 HCA
- Butanedioic acid, mercapto-, diethyl ester (9CI) (CA INDEX NAME)

- L39 ANSWER 155 OF 155 HCA COPYRIGHT 2003 ACS
- 51:34805 Original Reference No. 51:6601h-i,6602a-d Reductones derived from 3,4-dihydroxy-2,5-dicarboxylic esters of furan, thiophene, N-phenylpyrrole, and selenophene. v. Euler, Hans; Hasselquist, Hans (Univ. Stockholm). Z. physiol. chem., Hoppe-Seyler's, 306, 49-55 (Unavailable) 1956.
- For diagram(s), see printed CA Issue. GI
- cf. C.A. 49, 14844a. Compds. having the general structure MeO2CC:C(OH).C(OH):C(CO2Me).R (I) where R is O, S, Se, or Ph, were found to undergo ring cleavage under conditions ranging from soln. in warm H2O to heating with weakly alk. solns. or treatment with Tillmans reagent to give products having the general structure [MeO2CC(RH):C(OH)]2 (II). Di-Me 3,4-dihydroxyfuran-2,5-dicarboxylate (I, R, = O), .lambda. 282.5 m.mu. (8.15 .gamma./ml. in H2O) (log .epsilon. 4.25), gave no reaction with AcOH-phenylhydrazine but gave a di-Ac deriv. m. 141.degree. and was

oxidized by iodine soln, to a product that gave yellowish red crystals with phenylhydrazine, m. 130-2.degree.. On treatment of the ester with an equiv. of alkali, a salt was obtained. The salt or the ester gave 3,4-dihydroxyfuran-2-carboxylic acid, m. 139.degree. (decompn. with gas evolution), on heating in the absence of air with 2N NaOH. The effect of the ring-cleavage product, di-Me 2,3,4,5-tetrahydroxy-2,4-hexadienedioate (II, R = 0), on the viscosity of a pectin soln. was measured and compared to the similar effect of ascorbic acid. Di-Me 3,4-dihydroxythiophene-2,5-dicarboxylate (I, R = S), m. 174.degree. (di-Ac deriv., m. 105.5-6.5.degree.), on ring cleavage in alk. soln. gave di-Me 2,3,4-trihydroxy-5-thiol-2,4-hexadienedioate (II, R = S). Di-Me N-phenyl-3, 4-dihydroxypyrrole-2, 5-dicarboxylate (I, R = NPh), m.192.degree. (di-Ac deriv., m. 188.degree.), underwent ring cleavage to di-Me 2,3,4-trihydroxy-5-anilino-2,4-hexadienedioate (II, R = NPh). The di-Et deriv. of di-Me 3,4-dihydroxyselenophene-2,5-dicarboxylate (I, R = Se) was prepd. by satg. 4.5 g. NaOH in 10 ml. H2O with H2Se, adding 19 g. C1CH2CO2H, 20 g. Na2CO3, and 10 ml. H2O, then adding 22 g. concd. H2SO4 after 1 hr., heating, evapg. to dryness, extg. with MeOH, sepg. the salt, dilg. with H2O, and extg. with C6H6. Di-Me selenodiglycolate (1.6 g.), bl 129-30.degree. was treated with 1.5 g. di-Et oxalate and 0.75 g. Na in 15 ml. MeOH. Treatment with coned. HCl and recrystn. from EtOH gave 0.75 g. di-Me 3,4-diethoxyselenophene-2,5-dicarboxylate, m. 209.degree. Treatment with Ac20 gave di-Me 3,4-diacetoxyfuran-2,5-dicarboxylate, m. 141.degree.. The selenophene ring was unstable, and cleaved in H2O at 50.degree. to di-Me 2,3,4-trihydroxy-5-selenyl-2,4-hexadienedioate (II, R = Se). All the ring-cleavage products displayed biol. activity, inhibiting germination, mitosis, and the development of the Yoshida-Ascites carcinoma in rats. They decreased the viscosity of pectin and mucoid solns. and increased the permeability of cells.

TT 108754-29-6, Muconic acid, 2,3,4-trihydroxy-5-mercapto-, dimethyl ester

(prepn. of) ŔN 108754-29-6 HCA

CN Muconic acid, 2,3,4-trihydroxy-5-mercapto-, dimethyl ester (6CI) (CA INDEX NAME)

=> d L98 1-12 cbib abs hitind hitstr

L98 ANSWER 1 OF 12 HCA COPYRIGHT 2003 ACS 137:170401 Organic thiol, metal-free stabilizers and plasticizers for halogen-containing polymers. Starnes, William Herbert; Du, Bin (The College of William & Mary, USA). U.S. Pat. Appl. Publ. US 2002115769 A1 20020822, 12 pp., Cont.-in-part of U.S. Ser. No. 737,973. (English). CODEN: USXXCO. APPLICATION: US 2001-884306 20010619. PRIORITY: US 2000-737973 20001215.

AB (HS) zR3[CO2R4(SH)y]x and (HS) zR3[OCOR4(SH)y]x (R3, R4 = C1-20 hydrocarbyl,y, z = 0-10, x = 1-10) are useful as heat stabilizers and plasticizers for halopolymers giving compns. free of strong offensive odors. A typical compn. contained Oxyvinyls 455F (PVC) 100, HS(CH2)6OCO(CH2)4CO2(CH2)6SH 35, and stearic acid 0.1 part.

IC ICM C08K005-36

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TCS C11D001-28
     524316000
NCL
     37-6 (Plastics Manufacture and Processing)
     halopolymer aliph thiol ester odorless heat stabilizer
     ; PVC bismercaptohexyl adipate heat stabilizer
TT
     Heat stabilizers
       Plasticizers
        (odorless, org. thiol, metal-free stabilizers and plasticizers
        for halogen-contg. polymers)
     Chlorinated natural rubber
     RL: POF (Polymer in formulation); USES (Uses)
        (odorless, org. thiol, metal-free stabilizers and plasticizers
        for halogen-contg. polymers)
     Natural rubber, uses
IΤ
     RL: POF (Polymer in formulation); USES (Uses)
        (rubber hydrochloride; odorless, org. thiol, metal-free stabilizers and
        plasticizers for halogen-contq. polymers)
ΙT
     Esters, preparation
     RL: IMF (Industrial manufacture); MOA (Modifier or additive use); PREP
     (Preparation); USES (Uses)
        (thiol; odorless, org. thiol, metal-free stabilizers and
        plasticizers for halogen-contq. polymers)
IT
     9002-86-2, PVC
     RL: POF (Polymer in formulation); PRP (Properties); USES (Uses)
        (OxyVinyls 455F; odorless, org. thiol, metal-free stabilizers and
        plasticizers for halogen-contg. polymers)
     115-77-5, Pentaerythritol, reactions
ΙT
                                           1633-78-9, 6-Mercapto-1-hexanol
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (additive precursor; odorless, org. thiol, metal-free stabilizers and
        plasticizers for halogen-contg. polymers)
TT
     65291-46-5P, Bis(2-ethylhexyl) mercaptosuccinate 70537-68-7P,
     Pentaerythritol tetrakis(2-mercaptopropionate) 416900-24-8P,
     Bis(6-mercaptohexyl)adipate
     RL: IMF (Industrial manufacture); MOA (Modifier or additive use); PREP
     (Preparation); USES (Uses)
        (odorless, org. thiol, metal-free stabilizers and plasticizers
        for halogen-contg. polymers)
ΙT
     9002-85-1, Polyvinylidene chloride 9002-86-2D, PVC,
     chlorinated 9002-88-4D, Polyethylene,
     chlorinated 9003-53-6D, Polystyrene, chlorinated
     9010-98-4, Polychloroprene 25951-54-6, Polyvinyl
              51736-72-2, Polyvinylidene bromide
     RL: POF (Polymer in formulation); USES (Uses)
        (odorless, org. thiol, metal-free stabilizers and plasticizers
        for halogen-contg. polymers)
ΙT
     9002-86-2, PVC
     RL: POF (Polymer in formulation); PRP (Properties); USES (Uses)
        (OxyVinyls 455F; odorless, org. thiol, metal-free stabilizers and
        plasticizers for halogen-contg. polymers)
     9002-86-2 HCA
RN
     Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME)
CN
     CM
          1
     CRN
         75-01-4
          C2 H3 C1
     CMF
H2C= CH-C1
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70537-68-7P, Pentaerythritol tetrakis(2-mercaptopropionate)
IT
     416900-24-8P, Bis(6-mercaptohexyl)adipate
     RL: IMF (Industrial manufacture); MOA (Modifier or additive use); PREP
     (Preparation); USES (Uses)
        (odorless, org. thiol, metal-free stabilizers and plasticizers
        for halogen-contg. polymers)
RN
     70537-68-7 HCA
CN
     Propanoic acid, 2-mercapto-, 2,2-bis[(2-mercapto-1-oxopropoxy)methyl]-1,3-
     propanediyl ester (9CI) (CA INDEX NAME)
    SH O
Me-CH-C-O-CH2-C-CH2-O-C
                            O SH
        SH O
     416900-24-8 HCA
RN
     Hexanedioic acid, bis(6-mercaptohexyl) ester (9CI) (CA INDEX NAME)
CN
HS-(CH<sub>2</sub>)<sub>6</sub>-O-C-(CH<sub>2</sub>)<sub>4</sub>-C-O-(CH<sub>2</sub>)<sub>6</sub>-SH
IT 9002-86-2D, PVC, chlorinated-9002-88-4D,
     Polyethylene, chlorinated 9003-53-6D,
     Polystyrene, chlorinated 9010-98-4, Polychloroprene
     RL: POF (Polymer in formulation); USES (Uses)
        (odorless, org. thiol, metal-free stabilizers and plasticizers
        for halogen-contg. polymers)
     9002-86-2 HCA
RN
     Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME)
CN
     CM
          1
     CRN 75-01-4
     CMF C2 H3 C1
H_2C \longrightarrow CH - C1
ЯЯ
     9002-88-4 HCA
     Ethene, homopolymer (9CI) (CA INDEX NAME)
CN
     CM
          1
     CRN 74-85-1
     CMF C2 H4
H_2C = CH_2
RN
     9003-53-6 HCA
     Benzene, ethenyl-, homopolymer (9CI) (CA INDEX NAME)
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CM 1 CRN 100-42-5 CMF C8 H8 H2C== CH- Ph RN 9010-98-4 HCA CN 1,3-Butadiene, 2-chloro-, homopolymer (9CI) (CA INDEX NAME) CM 1 CRN 126-99-8 CMF C4 H5 C1 CH₂ C1-C-CH==CH2 L98 ANSWER 2 OF 12 HCA COPYRIGHT 2003 ACS 137:34042 Organic thiol metal-free stabilizers and plasticizers for halogen-containing polymers, especially poly(vinyl chloride). Starnes, William H., Jr.; Du, Bin (The College of William and Mary, USA). PCT Int. MITHAM H., JT.; DU, BIN (The College of William and Mary, USA). PCT 1
Appl. WO 2002048250 A2 20020620, 50 pp. DESIGNATED STATES: W: AE, AG,
AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ,
DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN,
IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK,
MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL,
TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2001-US48086 20011214. PRIORITY: US 2000-737973 20001215; US 2001-884306 20010619. Compds. R602CR5(SH)uCO2R7 (R5-7 = straight or branched hydrocarbyl of 1-20 AB C atoms; u = 1-20) are used in polymers normally susceptible to deterioration and color change, which typically occurs during processing of the polymer or exposure to certain environments. An intimate mixt. of PVC and di(2-ethylhexyl) 5-mercapto isophthalate (0.044 mol) was heated under Ar at 170.degree. for 1.5 h and at the end of the heating period, the mixt. retained its initial white color. IC ICM C08K005-00 37-6 (Plastics Manufacture and Processing) CC ST thiol heat stabilizer plasticizer IT Discoloration prevention agents Heat stabilizers Plasticizers (org. thiol metal-free stabilizers and plasticizers for halogen-contg. polymers, esp. poly(vinyl chloride)) ΙT Neoprene rubber, uses RL: POF (Polymer in formulation); USES (Uses) (org. thiol metal-free stabilizers and plasticizers for halogen-contg. polymers, esp. poly(vinyl chloride)) IΤ 9010-98-4 RL: POF (Polymer in formulation); USES (Uses) (neoprene rubber, org. thiol metal-free stabilizers and

plasticizers for halogen-contg. polymers, esp. poly(vinyl

RL: MOA (Modifier or additive use); USES (Uses)
 (plasticizers, vinyl chloride polymer compns. contg., with
 good radiation resistance)

IT 60-24-2 96-27-5, 3-Mercapto-1,2-propanediol 112-55-0, Dodecylmercaptan 123-81-9, Ethylene glycol bis(mercaptoacetate) 557-05-1, Zinc stearate 1191-08-8, 1,4-Dimercaptobutane 1592-23-0 2452-01-9, Zinc laurate 4696-56-4, Calcium laurate 7539-05-1, Pentaerythritol bis(.beta.-mercaptopropionate) 7634-42-6, 1,4-Dimercapto-2,3-butanediol 10193-95-0, 1,4-Butanediol bis(mercaptoacetate) 10193-96-1, Trimethylolpropane tris(mercaptoacetate) 20142-85-2, 3-Methoxy-2-hydroxypropylmercaptan 24431-38-7, 2-Hydroxyoctylmercaptan 25807-94-7, 2-Hydroxybutylmercaptan 33377-77-4, Dipentaerythritol tetrakis(mercaptoacetate) 73303-88-5 111532-30-0, 3-Octoxy-2-hydroxypropylmercaptan 132252-77-8, 3-Octylthio-2-hydroxypropylmercaptan 132405-61-9, Propylene glycol mono-.beta.-mercaptopropionate 132899-16-2 RL: USES (USES)

(vinyl chloride polymer compns. contg., with good radiation resistance)
IT 123-81-9, Ethylene glycol bis(mercaptoacetate) 7539-05-1
, Pentaerythritol bis(.beta.-mercaptopropionate) 10193-95-0,
1,4-Butanediol bis(mercaptoacetate) 10193-96-1,
Trimethylolpropane tris(mercaptoacetate)

Trimethylolpropane tris(mercaptoacetate)
RL: USES (Uses)

(vinyl chloride polymer compns. contg., with good radiation resistance)
RN 123-81-9 HCA
CN Acetic acid, mercapto-, 1,2-ethanediyl ester (9CI) (CA INDEX NAME)

RN 7539-05-1 HCA

RN 10193-95-0 HCA

CN Acetic acid, mercapto-, 1,4-butanediyl ester (9CI) (CA INDEX NAME)

RN 10193-96-1 HCA

CN Acetic acid, mercapto-, 2-ethyl-2-[[(mercaptoacetyl)oxy]methyl]-1,3propanediyl ester (9CI) (CA INDEX NAME)

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HS-CH2-C-O-CH2-C-Et O
                 CH2-O-C-CH2-SH
L98 ANSWER 5 OF 12 HCA COPYRIGHT 2003 ACS
103:216337 Thermal stabilization of vinyl chloride
    polymers. Gay, Michel (Rhone-Poulenc Specialites Chimiques, Fr.). Fr.
     Demande FR 2552440 A1 19850329, 46 pp. (French). CODEN: FRXXBL.
    APPLICATION: FR 1983-15745 19830928.
    Mixts. of org. Zn compds., org. compds. of Group IIA metals, and
AB
    2-mercaptopropionate esters are heat stabilizers for
    vinyl chloride polymers with little unpleasant odor. Thus,
    plasticized PVC [9002-86-2] (Corvic S 71/102)
    contg. Zn 2-ethylhexanoate [136-53-8] 1, Ba p-tert-butylbenzoate
     [10196-68-6] 0.5, and 2-ethylhexyl 2-mercaptopropionate (I) [99253-90-4]
    0.8 phr required 71 min to blacken at 180.degree., compared with 63 min
    with 0.2 phr I and 53 min with no I.
IC
    ICM C08K005-00
    ICS C08K005-37; C08J005-00; C08L027-06
CC
    37-6 (Plastics Manufacture and Processing)
    heat stabilizer PVC; zinc ethylhexanoate
    heat stabilizer; barium butylbenzoate heat
    stabilizer; mercaptopropionate ethylhexyl heat
    stabilizer
TT
    Heat stabilizers
        (alk. earth carboxylate-zinc carboxylate-mercaptopropionate ester
       mixts., with low odor, for PVC)
TΤ
    Alkaline earth compounds
    RL: USES (Uses)
        (carboxylates, heat stabilizers for PVC)
ΙT
    9002-86-2
    RL: USES (Uses)
        (heat stabilizers for, alk. earth org. compd.-zinc
       org. compd.-mercaptopropionate ester mixts. as, with low odor)
    136-53-8 526-26-1 557-04-0 557-05-1 1592-23-0 4980-54-5
ΙT
    6865-35-6 7529-07-9 10196-68-6 16850-01-4 17369-34-5
    27309-96-2 29367-13-3 52509-84-9 70537-67-6
                              99253-91-5 99253-92-6
    85892-79-1 99253-90-4
                              99253-95-9 99253-96-0
                                                        99253-97-1
                99253-94-8
    99253-93-7
                                           99254-01-0
                                                       99254-02-1
     99253-98-2
                99253-99-3
                              99254-00-9
    99254-03-2 99254-04-3 99254-05-4 99254-06-5
    99254-07-6 99254-08-7 99254-09-8
                              99254-12-3
                                           99254-13-4
                                                        99254-14-5
                 99254-11-2
    99254-10-1
                 99254-16-7
                              99254-17-8
                                          99254-18-9 99254-19-0
     99254-15-6
    99254-20-3 99270-47-0
    RL: MOA (Modifier or additive use); USES (Uses)
        (heat stabilizers, for PVC)
ΙT
    9002-86-2
    RL: USES (Uses)
        (heat stabilizers for, alk. earth org. compd.-zinc
        org. compd.-mercaptopropionate ester mixts. as, with low odor)
RN
    9002-86-2 HCA
    Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME)
CN
```

CM 1

CRN 75-01-4 CMF C2 H3 C1

H2C== CH- C1

IT 27309-96-2 70537-67-6 99253-92-6 99253-93-7 99254-04-3 99254-05-4 99254-06-5 99254-07-6 99254-08-7 99254-09-8 99254-10-1 99254-19-0

99254-20-3 99270-47-0

RL: MOA (Modifier or additive use); USES (Uses)

(heat stabilizers, for PVC)

RN 27309-96-2 HCA

CN Propanoic acid, 2-mercapto-, 1,2-ethanediyl ester (9CI) (CA INDEX NAME)

RN 70537-67-6 HCA

CN Propanoic acid, 2-mercapto-, 2-ethyl-2-[(2-mercapto-1-oxopropoxy)methyl]1,3-propanediyl ester (9CI) (CA INDEX NAME)

RN 99253-92-6 HCA

CN Propanoic acid, 2-mercapto-, 2,2-dimethyl-1,3-propanediyl ester (9CI) (CA INDEX NAME)

RN 99253-93-7 HCA

CN Propanoic acid, 2-mercapto-, 2,2-dimethyl-1-(1-methylethyl)-1,3propanediyl ester (9CI) (CA INDEX NAME)

RN 99254-04-3 HCA

CN Propanoic acid, 2-mercapto-, 1-methyl-1,2-ethanediyl ester (9CI) (CA INDEX NAME)

RN 99254-05-4 HCA

CN Propanoic acid, 2-mercapto-, 1,3-propanediyl ester (9CI) (CA INDEX NAME)

RN 99254-06-5 HCA

CN Propanoic acid, 2-mercapto-, 1-ethyl-1,2-ethanediyl ester (9CI) (CA INDEX NAME)

RN 99254-07-6 HCA

CN Propanoic acid, 2-mercapto-, 1,4-butanediyl ester (9CI) (CA INDEX NAME)

RN 99254-08-7 HCA

CN Propanoic acid, 2-mercapto-, 1,6-hexanediyl ester (9CI) (CA INDEX NAME)

RN 99254-09-8 HCA

RN 99254-10-1 HCA

CN Propanoic acid, 2-mercapto-, 2-ethyl-1-propyl-1,3-propanediyl ester (9CI)

John Calve, EIC - 1700, 308-4139

(CA INDEX NAME)

99254-19-0 HCA RN Propancic acid, 2-mercapto-, 2-[(2-mercapto-1-oxopropoxy)methyl]-2-methyl-1,3-propanediyl ester (9CI) (CA INDEX NAME)

RN 99254-20-3 HCA CN Propanoic acid, 2-mercapto-, 1,2,6-hexanetriyl ester (9CI) (CA INDEX

RN 99270-47-0 HCA CN Propanoic acid, 2-mercapto-, 1-methyl-1,3-propanediyl ester (9CI) (CA INDEX NAME)

L98 ANSWER 6 OF 12 HCA COPYRIGHT 2003 ACS 101:56557 Bonding dissimilar synthetic polymeric materials. Kwart, Harold; Varadhachary, Seevaram N. (USA). U.S. US 4333987 A 19820608, 9 pp. (English). CODEN: USXXAM. APPLICATION: US 1979-105051 19791219.

AB Adhesion between dissimilar polymers, esp. between vinyl polymers and photocurable polyurethane acrylates, is increased by adding plasticizers, nonvolatile, unsatd. compds., and radical initiators to the vinyl polymer and polythiols to the polyurethane and curing the pair in contact. Thus, a gelled PVC [9002-86-2] plastisol foam was printed with a vinyl polymer ink contg. a foaming inhibitor (trimellitic anhydride), covered with 15 mil wet PVC plastisol

```
contg. 5.0 phr glycerol diundecenoate [91115-16-1] and 0.3 phr Bz202,
      gelled at 300.degree. F, foamed at 430.degree. F, and coated with 1.5 mil
      mixt. of UV-curable polyurethane acrylate [dicyclohexylmethane
      diisocyanate (I) 3, 2-hydroxyethyl acrylate (II) 0.9, and
      polyoxypropylated pentaerythritol (III) 0.9 equivs.] 26.0, polyurethane
      acrylate (I 4 and II 2.4 equivs.) 4.4, III (OH no. 374) 4.6 and vinyl
      acetate 15.0 g contg. 2.5 g pentaerythritol tetrakis(mercaptoacetate)
      10193-99-4], 1.5 mL benzoin iso-Bu ether, and 5 drops Bu2Sn
      dilaurate. curing at 10 ft/min by two 200-W Hg lamps resulted in strong,
      permanent layer bonding.
· IC
      B05D003-06
 NCL
      428419000
      42-3 (Coatings, Inks, and Related Products)
CC
      adhesion PVC polyurethane acrylate; mercaptoacetate
      pentaerythritol coating adhesion; glycerol undecenoate coating adhesion
      Urethane polymers, uses and miscellaneous
TΨ
      RL: USES (Uses)
         (acrylates, bonding to PVC, polythiol-polyene couplers for)
ΙT
      Coupling agents
         (polythiol-polyenes, for photocurable polyurethane acrylates to
         PVC)
TΤ
     Oils
     RL: USES (Uses)
         (drying, couplers, contg. polythiols, for PVC to photocurable
         polyurethane acrylates)
IT
     Coating materials
         (photocurable, polyurethane acrylates, bonding to PVC,
         polyene-polythiol couplers for)
ΙT
     Thiols, uses and miscellaneous
     RL: USES (Uses)
         (poly-, couplers, contg. polyenes, for PVC to photocurable
        polyurethane acrylates)
IT
     10193-96-1 10193-98-3 10193-99-4
     68865-56-5
     RL: USES (Uses)
         (couplers, contg. polyenes, for PVC to photocurable
        polyurethane acrylates)
TΤ
     105-76-0
                91115-16-1
     RL: USES (Uses)
         (couplers, contg. polythiols, for PVC to photocurable
        polyurethane acrylates)
IΤ
     10193-96-1 10193-98-3 10193-99-4
     68865-56-5
     RL: USES (Uses)
        (couplers, contg. polyenes, for PVC to photocurable
        polyurethane acrylates)
RN
     10193-96-1 HCA
CN
     Acetic acid, mercapto-, 2-ethyl-2-[[(mercaptoacetyl)oxy]methyl]-1,3-
     propanediyl ester (9CI) (CA INDEX NAME)
```

RN 10193-98-3 HCA

CN Acetic acid, mercapto-, 2-[[(mercaptoacetyl)oxy]methyl]-2-methyl-1,3propanediyl ester (9CI) (CA INDEX NAME)

RN 10193-99-4 HCA

CN Acetic acid, mercapto-, 2,2-bis[[(mercaptoacetyl)oxy]methyl]-1,3propanediyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{O} & \text{CH}_2\text{--}\text{O}-\text{C}\text{--}\text{CH}_2\text{--}\text{SH} \\ | | \\ \text{HS--}\text{CH}_2\text{--}\text{C}-\text{O}-\text{CH}_2\text{--}\text{C}-\text{CH}_2\text{--}\text{O}-\text{C}-\text{CH}_2\text{--}\text{SH} \\ | \\ \text{HS--}\text{CH}_2\text{--}\text{C}-\text{O}-\text{CH}_2 & \text{O} \\ | | \\ \text{O} \end{array}$$

RN 68865-56-5 HCA

CN Poly(oxy-1,2-ethanediyl), .alpha.-(mercaptoacetyl)-.omega.[(mercaptoacetyl)oxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \mathsf{CH_2-CH_2-CH_2-CH_2-SH} \end{array}$$

L98 ANSWER 7 OF 12 HCA COPYRIGHT 2003 ACS

99:159565 Studies on treatment and effective utilization of polymer waste. V. Effect of thiol compounds on upgrading of scrap plasticized poly(vinyl chloride) hothouse film. Yamamoto, Makoto; Kawamoto, Kiyoshi; Yamaguchi, Tatsuaki (Tokyo Metrop. Ind. Tech. Inst., Tokyo, 115, Japan). Kobunshi Ronbunshu, 40(6), 345-50 (Japanese) 1983. CODEN: KBRBA3. ISSN: 0386-2186.

AB Poly(vinyl chloride) (I) [9002-86-2] resin was recovered from waste hothouse film by complete extn. of plasticizer with benzene at room temp. A disadvantage of recovered I is its lack of thermal stability, and resultant discoloration. Some improvement was obtained when an appropriate amt. of tris(mercaptopropyl) isocyanurate (II) [78366-85-5] was mixed into recovered I. The tensile strength of the material increased with the ratio of II to I. A strength of 59.3 N/mm2 was obtained when 5% II (based on I) was added. I was crosslinked with II in presence of dicumyl peroxide, but no addnl. improvement of properties resulted. II was a more effective additive for improving reclaimed I properties than 6-dibutylamino-1,3,5-triazine-2,4-dithiol [29529-99-5], pentaerythritol tetrakis(mercaptopropionate) [7575-23-7], isooctyl thioglycolate [25103-09-7], or diphenylthiourea [102-08-9].

CC 38-3 (Plastics Fabrication and Uses)

Section cross-reference(s): 60

ST PVC waste recovery upgrading; heat stabilizer

thiol recovered PVC; discoloration inhibiter thiol recovered RVC; mercaptopropyl isocyanurate stabilizer recovered PVC

IT Waste solids

TΤ

(PVC, recovered, thiol heat stabilizers

for)

Thiols, uses and miscellaneous

RL: MOA (Modifier or additive use); USES (Uses)

(heat stabilizers, for recovered PVC)

IT Heat stabilizers

(thiols, for PVC recovered from waste hothouse film)

IT Discoloration prevention

(agents, thiols, for PVC recovered from waste hothouse film)

IT Polymer degradation

(thermal, of recovered PVC, thiol stabilizers effect on)

IT 102-08-9 **7575-23-7** 25103-09-7 29529-99-5 78366-85-5

RL: MOA (Modifier or additive use); USES (Uses)

(heat stabilizers, for recovered PVC)

IT 9002-86-2

RL: USES (Uses)

(waste, stabilizers for recovered, thiols as)

IT 7575-23-7

RL: MOA (Modifier or additive use); USES (Uses)

(heat stabilizers, for recovered PVC)

RN 7575-23-7 HCA

CN Propanoic acid, 3-mercapto-, 2,2-bis[(3-mercapto-1-oxopropoxy)methyl]-1,3propanediyl ester (9CI) (CA INDEX NAME)

IT 9002-86-2

RL: USES (Uses)

(waste, stabilizers for recovered, thiols as)

RN 9002-86-2 HCA

CN Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 75-01-4

CMF C2 H3 C1

H2C== CH-C1

L98 ANSWER 8 OF 12 HCA COPYRIGHT 2003 ACS 98:216385 Reclamation of waste PVC film in agriculture. Yamamoto,

Makoto; Yamaguchi, Tatsuaki (Org. Chem. Div., Ind. Eng. Cent., Tokyo, 115, Japan). Enbi to Porima, 23(1), 7-11 (Japanese) 1983. CODEN: EBTPBO.

ISSN: 0367-021X.

The yield of reclaimed DOP [117-81-7] from waste soft PVC was AB 85.9, 93.6 and 86% for extn. at 20-30 .degree.C by benzene, toluene or 40:60 vol. MEK-MeOH mixt., resp. Acid value of the recovered DOP was lowered from 6.38 to 0.78 by treatment with active carbon and acidic alumina. Tensile strength of the residual PVC [9002-86-2] increased from 53.8 to 57.2 MPa by crosslinking with pentaerythritol tetra(3-mercaptopropionate) [7575-23-7]. The value increased to 58.0-60.0 MPa by using a coagent such as benzoyl peroxide [94-36-0]. Crosslinking reactions of PVC using typical thiol compds. are reviewed with 19 refs.

37-1 (Plastics Manufacture and Processing)

ST DOP recovery waste PVC; PVC waste crosslinking

IT Plasticizers

CC

(DOP, recovery of, from waste PVC)

IT Crosslinking catalysts

(benzoyl peroxide, for PVC)

IT Crosslinking agents

(pentaerythritol tetra(mercaptopropionate), for waste PVC)

ΙT 7575-23-7

RL: MOA (Modifier or additive use); USES (Uses)

(crosslinking agents, for waste PVC)

94-36-0, uses and miscellaneous

RL: CAT (Catalyst use); USES (Uses) (crosslinking catalysts, for PVC)

9002-86-2P ΙT

RL: PREP (Preparation)

(plasticizer recovery from waste)

TΤ 117-81-7P

RL: PREP (Preparation)

(recovery of, from waste PVC)

ΤТ 7575-23-7

RL: MOA (Modifier or additive use); USES (Uses)

(crosslinking agents, for waste PVC)

RN 7575-23-7 HCA

Propanoic acid, 3-mercapto-, 2,2-bis[(3-mercapto-1-oxopropoxy)methyl]-1,3-CN propanediyl ester (9CI) (CA INDEX NAME)

L98 ANSWER 9 OF 12 HCA COPYRIGHT 2003 ACS

96:144070 Recovery of plasticizer and crosslinked poly(vinyl chloride) (PVC) from waste agricultural soft film. Yamaguchi, Tatsuaki; Yamamoto, Makoto; Shimada, Yoshifusa (Dep. Ind. Chem., Chiba Inst. Technol., Narashino, 275, Japan). Kobunshi Ronbunshu, 39(1), 29-34 (Japanese) 1982. CODEN: KBRBA3. ISSN: 0386-2186.

More than 90 wt.% bis(2-ethylhexyl) phthalate (I) [117-81-7], which remained intact in waste agricultural plasticized PVC [9002-86-2] after 1-yr usage, (about 35 wt% of the original value) was recovered by dissoln.-repptn. with DMF and MeOH. A 60:40 (vol.%)

MeOH-MeCOEt mixt, was also effective for rapid extn. of I at room temp, The recovered PVC was converted to a crosslinked polymer by treatment with pentaerythritol tetrakis(3-mercaptopropionate) 7575-23-7) in the presence of Bz202. The thermal stability of the crosslinked PVC was better than that of the virgin PVC, and their tensile strengths were almost identical. CC 38-3 (Plastics Fabrication and Uses) Section cross-reference(s): 19 PVC recovery agricultural film; DOP recovery agricultural film; ST ethylhexyl phthalate recovery PVC film; phthalate ethylhexyl PVC film; waste PVC recovery film; plasticizer phthalate recovery PVC film IT Clays, uses and miscellaneous Kieselguhr RL: USES (Uses) (adsorbents, in recovery of DOP from waste agricultural PVC film, discoloration in relation to) ΙT Waste solids (agricultural PVC film, recovery and recrosslinking of) IΤ Plasticizers (bis(ethylhexyl) phthalate, recovery of, from waste PVC film) ΙT Adsorbents (in DOP recovery from waste agricultural PVC film) ΙT 1344-28-1, uses and miscellaneous 7440-44-0, uses and miscellaneous 14807-96-6, uses and miscellaneous RL: USES (Uses) (adsorbents, in recovery of DOP from waste agricultural PVC film, discoloration in relation to) ΙT 7575-23-7 RL: RCT (Reactant); RACT (Reactant or reagent) (crosslinking by, of PVC recovered from waste agricultural film) ΙT 117-81-7P RL: PREP (Preparation) (recovery of, from waste agricultural PVC film, by dissoln.-repptn.) IΤ 7575-23-7 RL: RCT (Reactant); RACT (Reactant or reagent) (crosslinking by, of PVC recovered from waste agricultural film) 7575-23-7 HCA RN Propanoic acid, 3-mercapto-, 2,2-bis[(3-mercapto-1-oxopropoxy)methyl]-1,3-CN propanediyl ester (9CI) (CA INDEX NAME)

L98 ANSWER 10 OF 12 HCA COPYRIGHT 2003 ACS
77:35605 Shapable plasticized thermoplastic compositions.
 Davenport, Noel E. (Grace, W. R., and Co.). Brit. GB 1270114 19720412, 5

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pp. (English). CODEN: BRXXAA. APPLICATION: GB 1969-8001 19690213.
     Thermoplastic compns., useful as protective or decorative coatings and
AΒ
     films, were prepd. from poly(vinyl chloride) (I) [9002-86-2] or vinyl
     chloride-vinyl acetate copolymer [9003-22-9] and a polymerizable
     plasticizer, e.g. diallyl phthalate (II) [131-17-9], and a
     polythiol, e.g. pentaerythritol mercaptopropionate (III) [
     7575-23-7]. Thus, a plastisol contg. I 100, II 50, III 45, basic
     lead carbonate 5, benzophenone photosensitizer 0.5, and Azosol Black MA
     0.4 parts was spread on a steel plate to form a 0.51 mm thick film which
     was fluxed at 200.deg. for 3 min. The fluxed film was flexible, but on
     irradn. with uv light for 10 min became hard, tough, and
     abrasion-resistant. Pentaerythitol tetrakis(thioglycollate) [
     10193-99-4] and an allyl-terminated polyester were similarly used.
IC
     C08F; C09D; B44D
CC
     36-6 (Plastics Manufacture and Processing)
     PVC coating plasticizer; allyl plasticizer
ST
     PVC; thiol curing PVC; polythiol curing PVC
IT
     Plasticizers
        (allyl group-contg., in chloroethylene polymer coatings)
ΙT
     Polyesters, uses and miscellaneous
     RL: USES (Uses)
        (allyl-terminated, plasticizers, in chloroethylene polymer
        coatings)
ΙT
     Coating materials
        (chloroethylene polymers, contq. polymerisable plasticizers
        and polythiols)
ΙT
     9002-86-2 9003-22-9
     RL: TEM (Technical or engineered material use); USES (Uses)
        (coatings, contq. polymerisable plasticizers and polythiols)
TΤ
     7575-23-7 10193-99-4
     RL: USES (Uses)
        (in chloroethylene polymer coatings)
ΙT
     131-17-9
     RL: USES (Uses)
        (plasticizers, for chloroethylene polymer coatings)
     7575-23-7 10193-99-4
     RL: USES (Uses)
        (in chloroethylene polymer coatings)
RN
     7575-23-7 HCA
CN
     Propanoic acid, 3-mercapto-, 2,2-bis[(3-mercapto-1-oxopropoxy)methyl]-1,3-
    propanediyl ester (9CI) (CA INDEX NAME)
```

RN 10193-99-4 HCA

CN Acetic acid, mercapto-, 2,2-bis[[(mercaptoacetyl)oxy]methyl]-1,3propanediyl ester (9CI) (CA INDEX NAME)

L98 ANSWER 11 OF 12 HCA COPYRIGHT 2003 ACS 77:20806 Curable thermoplastic polymer compositions contain a plasticizer. Davenport, Noel E. U.S. US 3652733 19720328, 3 pp. (English). CODEN: USXXAM. APPLICATION: US 1970-10032 19700209. Poly(vinyl chloride) (I) [9002-86-2] and vinyl chloride-vinyl acetate AΒ copolymer [9003-22-9] were mixed with a polymerizable plasticizer such as pentaerythritol mercaptopropionate (II) [7575-23-7] or pentaerythritol tetrakisthioglycollate [10193-99-4] to give curable compns. useful as coatings. Thus, a plastisol, prepd. from Breon 121, diallyl phthalate, II (45%), basic Pb carbonate, benzophenone, and Azosol Black MA, was applied on a steel plate, fluxed at 200.deg., and exposed to uv light to give hard and abrasion resistant film. IC C08F NCL 260884000 CC 36-6 (Plastics Manufacture and Processing) PVC plastisol; UV crosslinking PVC; coating PVC; pentaerythritol mercaptopropionate plasticizer; thioglycollate plasticizer; polymerizable plasticizer PVC IT Plasticizers (mercapto acid pentaerythritol esters as polymerizable, for vinyl chloride polymer coatings for steel) TΤ Coating materials (vinyl chloride polymers, contq. polymerizable plasticizers, for steel) ΙT 9002-86-2 9003-22-9 RL: TEM (Technical or engineered material use); USES (Uses) (coatings, contg. polymerizable plasticizers, for steel) ΙT 7575-23-7 10193-99-4 RL: MOA (Modifier or additive use); USES (Uses) (plasticizers, polymerizable, for vinyl chloride polymers as

RN 7575-23-7 HCA

TT

CN Propanoic acid, 3-mercapto-, 2,2-bis[(3-mercapto-1-oxopropoxy)methyl]-1,3propanediyl ester (9CI) (CA INDEX NAME)

(plasticizers, polymerizable, for vinyl chloride polymers as

coatings for steel)

coatings for steel)

RL: MOA (Modifier or additive use); USES (Uses)

7575-23-7 10193-99-4

RN 10193-99-4 HCA

CN Acetic acid, mercapto-, 2,2-bis[[(mercaptoacetyl)oxy]methyl]-1,3propanediyl ester (9CI) (CA INDEX NAME)

L98 ANSWER 12 OF 12 HCA COPYRIGHT 2003 ACS
75:28230 Lithographic plate. Yeshin, Leon (Grace, W. R., and Co.). Fr.
Demande FR 2028302 19701113, 36 pp. (French). CODEN: FRXXBL. PRIORITY:
US 19690114.

AB Lithographic plates were made using a plastic or Al support coated with a photohardenable layer contg. a vinyl polymer and 2-98 parts polyene, 2-98 parts polythiol and 0.005-50 parts accelerator/100 parts polyene and polythiol. An image formed on uv irradn. through a diapos. or stencil, and the heated compn. contained insol., pliant exposed areas, and plasticized hydrophilic or oleophilic unexposed ones. Thus, a polymer prepd. from a polyester glycol treated with allyl isocyanate in the presence of dibutyl tin dilaurate was mixed with pentaerythritol tetrakis(.beta.-mercaptopropionate), benzophenone photoinitiator and PVC, heated, and coated on Al. Similar coating prepns. (85 given) contain other mercaptans and prepd. polymers, poly(vinylidene chloride) in place of PVC, and cyclohexanone, acetone or MeEt ketone photoinitiator, coated, e.g. on Mylar.

IC G03F; B41N; C08F

CC 74 (Radiation Chemistry, Photochemistry, and Photographic Processes)

IT 7575-23-7

RL: USES (Uses)

(photohardenable compns. contg., for lithographic plate)

IT 7575-23-7

RL: USES (Uses)

(photohardenable compns. contg., for lithographic plate)

RN 7575-23-7 HCA

CN Propanoic acid, 3-mercapto-, 2,2-bis[(3-mercapto-1-oxopropoxy)methyl]-1,3propanediyl ester (9CI) (CA INDEX NAME)

=> d L99 1,5,10,20,25,30,35,40-41 cbib abs hitstr

L99 ANSWER 1 OF 41 HCA COPYRIGHT 2003 ACS 137:80395 Heavy metal-free heat stabilizer compositions for water-based inks or other PVC resins with improved adhesion. Duvall, Tod C.; Carpenter, Jeffrey L. (USA). U.S. Pat. Appl. Publ. US 2002086920 Al 20020704, 15 pp., Cont.-in-part of U.S. Ser. No. 133,605. (English). CODEN: USXXCO. APPLICATION: US 1999-320304 19990526. PRIORITY: US 1995-435413 19950510; US 1996-597093 19960223; US 1997-890613 199/0709; US 1998-48492 19980326; US 1998-133605 19980813.

AB The compns. comprise a combination of a blocked mercaptan and a zinc salt of oxidized polyethylene (a zinc ionomer), wherein the oxidized polyethylene is split out from the ionomer to act as an adhesion promoter for ag. inks and paints, and the residual zinc carboxylate functions as a co-stabilizer with the mercaptan in the compn. One example of the mercaptans was 2-S-(tetrahydropyranyl)thioethyl caprate.

TΤ 9002-86-2, PVC

RL: POF (Polymer in formulation); PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

(heat stabilizer compns. for water-based inks or PVC resins with improved adhesion)

RN 9002-86-2 HCA

CN Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 75-01-4 CMF C2 H3 C1

 $H_2C = CH - C1$

IT 107571-76-6P, Pentaerythritol bis(2-mercaptoacetate) RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent) (intermediate; heat stabilizer compns. for water-based inks or PVC resins with improved adhesion) 107571-76-6 HCA RN Acetic acid, mercapto-, 2,2-bis(hydroxymethyl)-1,3-propanediyl ester (9CI) CN

(CA INDEX NAME)

L99 ANSWER 5 OF 41 HCA COPYRIGHT 2003 ACS

118:125812 Heat- and discoloration-resistant chlorinated PVC compositions. Oomoto, Masanobu; Kawamoto, Kazuo; Kakei, Hiroshi (Sekisui Chemical Co., Ltd., Japan; Tokuyama Soda Co., Ltd.). Jpn. Kokai Tokkyo Koho JP 04198348 A2 19920717 Heisei, 9 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1990-327331 19901127.

AΒ The title compns. comprise chlorinated PVC contg. 0.05-5 phr alkyltin compds. and 0.05-5 phr S- and/or Cl-contg. alkyltin compds. and/or metal halides. Thus, a molding prepd. by molding HA 15F contg. MBS (Metablen C 150S) 10, Hiwax 4202E, dioctyltin sulfide 2, and monooctyltin(isooctylmercaptoacetate) chloride (I) 1 phr at 180.degree. for 7 min had yellowness 33, vs. 43 without I.

ΙT 10193-96-1 10193-99-4, Pentaerythritol tetrakis (mercaptoacetate) 22504-50-3 92140-97-1 145821-74-5

RL: USES (Uses)

(chlorinated PVC contq. alkyltin compds. and, heat-resistant)

RN 10193-96-1 HCA

CN Acetic acid, mercapto-, 2-ethyl-2-[[(mercaptoacetyl)oxy]methyl]-1,3propanediyl ester (9CI) (CA INDEX NAME)

RN 10193-99-4 HCA

Acetic acid, mercapto-, 2,2-bis[[(mercaptoacetyl)oxy]methyl]-1,3-CN propanediyl ester (9CI) (CA INDEX NAME)

22504-50-3 HCA RN

Propanoic acid, 3-mercapto-, 1,2-ethanediyl ester (9CI) (CA INDEX NAME) CN

RN 92140-97-1 HCA

CN Propanoic acid, 3-mercapto-, 1,4-butanediyl ester (9CI) (CA INDEX NAME)

RN 145821-74-5 HCA

CN Propanoic acid, 3-mercapto-, 1-methyl-1,2-ethanediyl ester (9CI) (CA INDEX NAME)

L99 ANSWER 10 OF 41 HCA COPYRIGHT 2003 ACS

114:144830 Thermal stabilization of chlorinated PVC. Adachi,
Terufumi; Kakei, Hiroshi; Kawamoto, Kazuo (Tokuyama Sekisui Industry Co.,
Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 02269756 A2 19901105 Heisei, 8
pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1989-92228 19890411.

AB Chlorinated PVC is stabilized with mixts. of alkyltin chlorides and the thiols of specified structure. Thus, chlorinated PVC contg. 1.4 phr (C8H17)2Sn(Cl)SCH2CO2C8H17-iso and 0.6 phr HOCH2CH2SH had good stability at 190.degree. for 140 min.

IT 9002-86-2D, PVC, chlorinated

RL: USES (Uses)

(heat stabilizers for, alkyltin chlorides and

thiols as)

RN 9002-86-2 HCA

CN Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 75-01-4 CMF C2 H3 C1

H2C==CH-C1

IT 10193-99-4

RL: MOA (Modifier or additive use); USES (Uses) (heat stabilizers, for chlorinated PVC)

RN 10193-99-4 HCA

CN Acetic acid, mercapto-, 2,2-bis[[(mercaptoacetyl)oxy]methyl]-1,3-propanediyl ester (9CI) (CA INDEX NAME)

L99 ANSWER 20 OF 41 HCA COPYRIGHT 2003 ACS 98:126738 Mechanism of poly(vinyl chloride) stabilization by mixtures of zinc and calcium carboxylates with various complexing agents. Troitskii, B. B.; Troitskaya, L. S.; Denisova, V. N. (Inst. Chem., Gorskii, USSR). European Polymer Journal, 18(12), 1093-101 (English) 1982. CODEN: EUPJAG. ISSN: 0014-3057. AB The effects were studied at 180.degree. for Zn and Ca carboxylates, polyols, and other O-contg. compds., N- and S-contg. compds., and of mixts. of Zn-Ca carboxylates, Zn carboxylate-complexing agent, Ca carboxylate-complexing agent, and of Zn carboxylate-Ca carboxylate-complexing agent upon the rate of dehydrochlorination and crosslinking and on the absorption spectra of PVC during degrdn. in vacuum. The interaction of the stabilizers with 2-chlorobutane (a model for normal units of PVC [9002-86-2]) was studied at 180.degree.. In the thermal degrdn. of PVC, Zn carboxylates give synergistic mixts. with compds. having -OH, -SH, or -NH groups. In the thermal degrdn. of PVC in the presence of mixts. of Zn carboxylates with polyols, there are exchanges between Cl-contg. groups of PVC and COO- groups of salt and alc. residue. In salts also catalyze the interaction of polyols with double (particularly conjugated double) bonds of degraded PVC. The investigated compds. do not form synergistic mixts. with Ca carboxylates. The triple mixts. of Zn and Ca carboxylates with complexing agents are more effective stabilizers of PVC than the binary mixts. Zn carboxylate-Ca carboxylate and Zn carboxylate-complexing agent. The mechanism of synergistic interaction in PVC stabilization by these mixts. is discussed. 9002-86-2 RL: PRP (Properties) (degrdn. of, thermal, kinetics of, effect of stabilizers on) RN 9002-86-2 HCA CN Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME) CM 1 CRN 75-01-4 CMF C2 H3 C1

 $H_2C = CH - C1$

IT 123-81-9 RL: USES (Uses) (stabilizers, thermal degrdn. of PVC in presence of, kinetics RN 123-81-9 HCA CN Acetic acid, mercapto-, 1,2-ethanediyl ester (9CI) (CA INDEX NAME)

John Calve, EIC - 1700, 308-4139 Page 56

L99 ANSWER 25 OF 41 HCA COPYRIGHT 2003 ACS

97:56732 Improved stabilizers for vinyl halide resins.. Hulyalkar, Ramchandra K.; Baum, Gerald A.; Hotchandani, Kanayo (Dart and Kraft, Inc., USA). Belg. BE 891693 Al 19820430, 19 pp. (French). CODEN: BEXXAL. APPLICATION: BE 1982-206989 19820105. PRIORITY: US 1981-232108 19810206.

AR An ethoxylated organophosphate ester such as Gafac RS 410 [9046-01-9] or Gafac RE 610 [51811-79-1] is mixed with a liq. compd. contg. S and Sb, such as Sb(SCH2CO2R)3 (R = isooctyl) (I) [27288-44-4], to improve the hydrolysis resistance of the liq. compd. The liq. mixts. were used as heat stabilizers for PVC [9002-86-2

] and similar resins. Thus, a 98:2 I-Gafac RS 410 mixt. was resistant to hydrolysis during 108 min while humid air was passed through the liq. mixt. at 127.degree.. PVC contg. 0.8% of the mixt. became slightly colored during 20 min at 190.5.degree. and became brown-black during 45 min.

9002-86-2 ΙT

RL: USES (Uses)

(heat stabilizers for, antimony

mercaptide-ethoxylated organophosphate ester mixts. as)

9002-86-2 HCA RN

CN Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 75-01-4 CMF C2 H3 Cl

 $H_2C = CH - C1$

ΙT 82530-62-9

> RL: MOA (Modifier or additive use); USES (Uses) (heat stabilizers, for PVC, hydrolysis

inhibitors for)

82530-62-9 HCA RN

Acetic acid, mercapto-, 1,2-ethanediyl ester, antimony(3+) salt (3:1) CN (9CI) (CA INDEX NAME)

●1/3 Sb(III)

L99 ANSWER 30 OF 41 HCA COPYRIGHT 2003 ACS 94:47482 Organotin compounds and resins or polymers stabilized with them. Dworking, Robert Dally; Larkin, William Albert (M and T Chemicals Inc., USA). Eur. Pat. Appl. EP 11456 19800528, 101 pp. (English). CODEN: EPXXDW. APPLICATION: EP 1979-302520 19791109.

Szekely

GΙ

AB Approx. 20 organotin sulfide esters were prepd. by various procedures. Thus, 0.4 mol BuSnCl3, 0.8 mol NH4OH, 0.2 mol HSCH2CH2OH, 0.2 mol Me(CH2)11SH, 0.2 mol HSCH2CH2OZC(CH2)7CO2CH2CH2SH, and 233 mol H2O, was heated to 70.degree. 0.5 h by 0.2 mol Na2S addn., the mixt. heated at 75.degree. 0.5 h, and the pH adjusted to 7 with NH4OH to give 88 g I (R = n-dodecyl). Also prepd. were [(BuSn(S)SCH2CH2O]4M (M = Si, Ti), [BuSn(S)SCH2CH2O]3M (M = B, P, Al), and I (R = CH2CO2(CH2)5CHMe2). The compds. prepd. were useful as heat stabilizers for halogenated polymers such as FVC.

IT 9002-86-2

RN

RL: RCT (Reactant); RACT (Reactant or reagent)
 (organotin compds. as stabilizers for)
9002-86-2 HCA

Т

CN Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 75-01-4 CMF C2 H3 C1

 $H_2C = CH - C1$

IT 10194-00-0 76192-65-9

RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with butyltin chlorides)

RN 10194-00-0 HCA

CN Hexanedioic acid, bis(2-mercaptoethyl) ester (9CI) (CA INDEX NAME)

RN 76192-65-9 HCA

CN Nonanedioic acid, bis(2-mercaptoethyl) ester (9CI) (CA INDEX NAME)

L99 ANSWER 35 OF 41 HCA COPYRIGHT 2003 ACS 86:56234 Organotin compounds. Coates, Harold; Collins, John Desmond;

Siddiqui, Iftikhar H. (Albright and Wilson Ltd., UK). Brit. GB 1439753 19760616, 15 pp. Division of Brit. 1,439,752. (English). CODEN: BRXXAA. APPLICATION: GB 1973-22460 19730510.

AR Improved stabilization of PVC against thermal decompn. was obtained using low Sn content bis[(alkyloxycarbonyl)ethylthio|dibutyl- and -diocytltin deriv. stabilizers. E.g., HS(CH2)2CO2CH2C(CH2O2CC11H23)3 [60998-31-4], prepd. by condensing pentaerythritol [115-77-5], lauric acid [143-07-7], and HS(CH2)CO2H [107-96-0] together, was treated with Bu2SnO [818-08-6] to give Bu2Sn[S(CH2)2CO2CH2C(CH2O2CC11H23)3]2 (I) [60998-27-8]. A rigid sample of Corvic D55/9 contg. 1.16 parts I/100 parts resin had Gardner Scale color 6 after 10 min at 190.degree. compared with a color 7 for a conventional Sn-stabilized PVC (Mellite 31C) contg. an equiv. amt. of stabilizer. Five other stabilizers were prepd.

45312-48-9P IΤ

RL: PREP (Preparation)

(prepn. and condensation reaction with dodecylaldehyde)

45312-48-9 HCA RN

Dodecanoic acid, 3-(3-mercapto-1-oxopropoxy)-2,2-bis[(3-mercapto-1-CN oxopropoxy)methyl]propyl ester (9CI) (CA INDEX NAME)

7575-23-7P IΤ

RL: PREP (Preparation)

(prepn. and condensation reaction with salicylaldehyde)

RN 7575-23-7 HCA

CN Propanoic acid, 3-mercapto-, 2,2-bis[(3-mercapto-1-oxopropoxy)methyl]-1,3propanediyl ester (9CI) (CA INDEX NAME)

TΤ 9002-86-2

RL: USES (Uses)

(stabilizers for, bis[(alkoxycarbonyl)ethylthio]dibutyltin derivs. as)

RN 9002-86-2 HCA

CN Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 75-01-4

Szekelv

CMF C2 H3 C1

HoC=CH-Cl

L99 ANSWER 40 OF 41 HCA COPYRIGHT 2003 ACS

71:72073 Pentaerythritol mercaptopropionate-modified vinyl chloride polymers. Hwa, Jesse C. H. (Stauffer Chemical Co.). S. African ZA 6805047 19690124, 30 pp. (English). CODEN: SFXXAB. PRIORITY: US 19670901.

Vinyl halide polymers contg. a polymercaptan (I) are prepd., which have AB exceptional thermal stability and low fluxing or flowing characteristics to allow for easier polymer processing without sacrificing phys. properties. The modified vinyl halide polymers have excellent solvent soly, and can be used as a soln, coating compn., which have increased adhesion to a substrate without sacrificing their phys. properties. Thus, a mixt. of vinyl chloride 100, water 230, I 0.3 (contg. 35%) pentaerythritol tetrakis (3-mercaptopropionate) and 35% pentaerythritoltris(3-mercaptopropionate)], hydroxymethyl cellulose 0.167, and azobisiso-butyronitrile 0.067 part was suspension polymd. for 14 hrs. at 44.degree. to give 1.89 relative viscosity (1 wt. % in cyclohexanone, 30.degree.) and a 95-100% conversion. A vinyl chloride polymer 100 contq. I 0.3, stabilizer 3, and lubricant (Ca stearate) 0.5 part had a fusion torque rheometer reading rating of noncatastrophic (polymer degrades at a rate of 0-25 m.-g./min.) and 8010 tensile strength, compared to semicatastrophic (polymers degrade at a rate of 25-100 m.-g./min.) and 7440 for a conventional low-mol.-wt. poly-(vinyl chloride) homopolymer, with the same amts. of the stabilizer lubricant but without I.

TΤ 7539-04-0 7575-23-7

RL: USES (Uses)

(polymn. of vinyl chloride in presence of, for coatings)

RN 7539-04-0 HCA

Propanoic acid, 3-mercapto-, 2-(hydroxymethyl)-2-[(3-mercapto-1-CN oxopropoxy)methyl]-1,3-propanediyl ester (9CI) (CA INDEX NAME)

7575-23-7 HCA RN

Propanoic acid, 3-mercapto-, 2,2-bis[(3-mercapto-1-oxopropoxy)methyl]-1,3-CN propanediyl ester (9CI) (CA INDEX NAME)

TT 9002-86-2P, preparation

RL: PREP (Preparation) (presence of pentaerythritol mercaptopropionate, for coatings) RN CN Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 75-01-4 CMF C2 H3 C1

H2C=CH-C1

L99 ANSWER 41 OF 41 HCA COPYRIGHT 2003 ACS 57:76105 Original Reference No. 57:15152e-h Organotin sulfur compounds. Mack, Gerry P. (Metal & Thermit Corp.). GB 9003068 19620809, 4 pp. (Unavailable). PRIORITY: US 19600401.

AB Organotin S compds., excellent stabilizers for the prevention of heat degradation in vinyl chloride-contg. resins, are prepd. by treating a diorganotin oxide (or its corresponding dihydroxide, dichloride, or dibromide) of the formula R2SnO, where R is a phenyl, alkyl, or aralkyl group contg. not more than 12 C atoms, with pentaerythritol tetramercaptoacetate or pentaerythritol tetra-.beta.-mereaptopropionate (or their sodium salts) in a molar ratio of 2 pts. of the oxide to 1 of the ester. The product is believed to have the formula [R2Sn]2[C(CH2OCO R'S)4] where R' is a methylene or an ethylene group. The reaction is usually carried out in an inert liquid, such as toluene, acetone, benzene, water, etc. Thus, 4.8 moles dibutyltin oxide is added to 2.4 moles pentaerythritol tetrakis (mercaptoacetate) in 8000 ml. toluene at 55.degree.. The mixt. is then heated to reflux and the water sepd. The reaction product ppts. as a white solid. This product is an excellent stabilizer for polyvinyl chloride resins when present in amts. of 0.5 to 2.5 parts/100 parts of resin. ΙŢ

10193-99-4, Pentaerythritol, tetrakis(mercaptoacetate)

(reaction products with dialkyloxotin derivs.)

RN 10193-99-4 HCA

CN

Acetic acid, mercapto-, 2,2-bis[[(mercaptoacetyl)oxy]methyl]-1,3propanediyl ester (9CI) (CA INDEX NAME)

- 1

CMF C2 H3 C1

H2C=CH-C1

L99 ANSWER 40 OF 41 HCA COPYRIGHT 2003 ACS

71:72073 Pentaerythritol mercaptopropionate-modified vinyl chloride polymers. Hwa, Jesse C. H. (Stauffer Chemical Co.). S. African ZA 6805047 19690124, 30 pp. (English). CODEN: SFXXAB. PRIORITY: US 19670901.

AB Vinyl halide polymers contq. a polymercaptan (I) are prepd., which have exceptional thermal stability and low fluxing or flowing characteristics to allow for easier polymer processing without sacrificing phys. properties. The modified vinyl halide polymers have excellent solvent soly, and can be used as a soln, coating compn., which have increased adhesion to a substrate without sacrificing their phys. properties. Thus, a mixt. of vinyl chloride 100, water 230, I 0.3 [contg. 35% pentaerythritol tetrakis (3-mercaptopropionate) and 35% pentaerythritoltris(3-mercaptopropionate)], hydroxymethyl cellulose 0.167, and azobisiso-butyronitrile 0.067 part was suspension polymd. for 14 hrs. at 44.degree. to give 1.89 relative viscosity (1 wt. % in cyclohexanone, 30.degree.) and a 95-100% conversion. A vinyl chloride polymer 100 contg. I 0.3, stabilizer 3, and lubricant (Ca stearate) 0.5 part had a fusion torque rheometer reading rating of noncatastrophic (polymer degrades at a rate of 0-25 m.-q./min.) and 8010 tensile strength, compared to semicatastrophic (polymers degrade at a rate of 25-100 m.-g./min.) and 7440 for a conventional low-mol.-wt. poly-(vinyl chloride) homopolymer, with the same amts. of the stabilizer lubricant but without I.

7539-04-0 7575-23-7 TT

RL: USES (Uses)

(polymn. of vinyl chloride in presence of, for coatings)

RN 7539-04-0 HCA

CN

Propanoic acid, 3-mercapto-, 2-(hydroxymethyl)-2-[(3-mercapto-1oxopropoxy)methyl]-1,3-propanediyl ester (9CI) (CA INDEX NAME)

RN 7575-23-7 HCA

Propanoic acid, 3-mercapto-, 2,2-bis[(3-mercapto-1-oxopropoxy)methyl]-1,3-CN propanediyl ester (9CI) (CA INDEX NAME)

9002-86-2P, preparation ΙT

RL: PREP (Preparation)

(presence of pentaerythritol mercaptopropionate, for coatings)

RN 9002-86-2 HCA

CN Ethene, chloro-, homopolymer (9CI) (CA INDEX NAME)

CM

CRN 75-01-4 CMF C2 H3 C1

H2C == CH - C1

L99 ANSWER 41 OF 41 HCA COPYRIGHT 2003 ACS 57:76105 Original Reference No. 57:15152e-h Organotin sulfur compounds. Mack, Gerry P. (Metal & Thermit Corp.). GB 9003068 19620809, 4 pp. (Unavailable). PRIORITY: US 19600401.

AB Organotin S compds., excellent stabilizers for the prevention of heat degradation in vinyl chloride-contg. resins, are prepd. by treating a diorganotin oxide (or its corresponding dihydroxide, dichloride, or dibromide) of the formula R2SnO, where R is a phenyl, alkyl, or aralkyl group contg. not more than 12 C atoms, with pentacrythritol tetramercaptoacetate or pentaerythritol tetra-.beta.-mereaptopropionate (or their sodium salts) in a molar ratio of 2 pts. of the oxide to 1 of the ester. The product is believed to have the formula [R2Sn]2[C(CH2OCO R'S)4] where R' is a methylene or an ethylene group. The reaction is usually carried out in an inert liquid, such as toluene, acetone, benzene, water, etc. Thus, 4.8 moles dibutyltin oxide is added to 2.4 moles pentaerythritol tetrakis (mercaptoacetate) in 8000 ml. toluene at 55.degree.. The mixt. is then heated to reflux and the water sepd. The reaction product ppts. as a white solid. This product is an excellent stabilizer for polyvinyl chloride resins when present in amts. of 0.5 to 2.5 parts/100 parts of resin. ΙT

10193-99-4, Pentaerythritol, tetrakis (mercaptoacetate)

(reaction products with dialkyloxotin derivs.)

10193-99-4 HCA RN

CN Acetic acid, mercapto-, 2,2-bis[[(mercaptoacetyl)oxy]methyl]-1,3propanediyl ester (9CI) (CA INDEX NAME)

=> d L117 1 cbib abs hitind hitstr

L117 ANSWER 1 OF 1 HCA COPYRIGHT 2003 ACS 110:174486 Process for stabilizing mixtures based on halogenated polymers. Kornbaum, Simon (Fr.). PCT Int. Appl. WO 8810282 Al 19881229, 23 pp. DESIGNATED STATES: W: AU, BG, BR, DK, FI, HU, JP, KR, MC, NO, RO, SU, US; RW: AT, BE, BJ, CF, CG, CH, CM, DE, FR, GA, GB, IT, LU, ML, MR, NL, SE,

SN, TD, TG. (French). CODEN: PIXXD2. APPLICATION: WO 1988-FR332 19880622. PRIORITY: FR 1987-9279 19870626.

- AB In the title process, .gtoreq.1 org. compds. contg. .gtoreq.1 SH groups and a small amt. of .gtoreq.1 halides selected from organometallic halides and/or metallic halides are added to the mixts. during their prepn. A compn. comprising Lacqvyl S 071 s (PVC) 100, BTA III F 7, AC 316 A (lubricant) 0.3, Lacer BN (lubricant) 0.45, epoxidized soybean oil 1, C(CH2O2CCH2SH)4 1, and n-C8H17SnCl3 (I) 0.017 part showed color stability 9 min and thermal stability 12 min, compared with .ltoreq.2 min and 4 min, resp., without I.

 IC ICM CO8K005-00
 - IC ICM C08K005-00 ICS C08K013-02; C08L027-02; C08L027-06
- ICI C08K005-00, C08K005-37, C08K005-56; C08K005-00, C08K005-37, C08K005-57; C08K013-02, C08K003-16, C08K005-37
- CC 37-6 (Plastics Manufacture and Processing)
- IT 3091-25-6 3542-36-7, Dioctyltin dichloride 7646-78-8, Tin tetrachloride, uses and miscellaneous 10108-64-2, Cadmium dichloride 10193-99-4, Pentaerythritol tetramercaptoacetate 26401-97-8 RL: USES (Uses)

(stabilizers, for halogenated polymer compns.)

IT 10193-99-4, Pentaerythritol tetramercaptoacetate RL: USES (Uses) (stabilizers, for halogenated polymer compns.)

RN 10193-99-4 HCA

CN Acetic acid, mercapto-, 2,2-bis[[(mercaptoacetyl)oxy]methyl]-1,3propanediyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{O} \\ \text{O} \\ \text{CH}_2-\text{O}-\text{C}-\text{CH}_2-\text{SH} \\ \text{HS}-\text{CH}_2-\text{C}-\text{O}-\text{CH}_2-\text{C}-\text{CH}_2-\text{O}-\text{C}-\text{CH}_2-\text{SH} \\ \text{HS}-\text{CH}_2-\text{C}-\text{O}-\text{CH}_2 \\ \text{O} \\ \end{array}$$

Peter, the answer are not great.

sogbean oil, adipie Lacid, claim 22...

=> d L115 1,5,10,15,20,25,30,35,40,45, 50, 55, 60,65,70-72 cbib abs hitind hitstr

L115 ANSWER 1 OF 72 HCA COPYRIGHT 2003 ACS

136:355810 Polyoxyalkylene mercapto fatty acid esters and their manufacture. Miyata, Katsuji; Kazutomo, Toshio; Tateishi, Hayami; Kawasaki, Noriaki; Nakamura, Naoya; Tsuboi, Makoto (Sakai Chemical Industry Co., Ltd., Japan; Chugoku Marine Paints, Ltd.). Jpn. Kokai Tokkyo Koho JP 2002128889 A2 20020509, 8 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 2000-325535 20001025.

The polyoxyalkylene monoesters or diesters with mercapto fatty acids shown as R10(R20) nCO(CH2)mSH [R1 = H, C1-20 alkyl, C2-20 alkenyl, C6-20 (substituted) Ph; R2 = C1-4 alkylene; l = m = 1-10; n = 1-30] or HS(CH2) lCO2(R20) nCO(CH2)mSH (R2 = C1-4 alkylene; l, m = 1-30; 3 < n .1toreq. 30) are manufd. by esterification of R10(R20)nH with HO2C(CH2)mSH or esterification of R10(R20)nH with HO2C(CH2)lSH. Thus, reaction of 5.01 mol 3-mercaptopropionic acid with 2.50 mol polyethylene glycol at 100-125.degree. for 5 h in the presence of p-toluenesulfonic acid gave 2.19 mol polyethylene glycol bis (3-mercaptopropionate).

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ICM C08G065-334
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37-3 (Plastics Manufacture and Processing)

Polyoxyalkylenes, preparation

RL: IMF (Industrial manufacture); PREP (Preparation)

(acrylic, block; manuf. of polyoxyalkylene mercapto fatty

acid esters for prepn. of block copolymer)

IT Polyoxyalkylenes, preparation

RL: IMF (Industrial manufacture); TEM (Technical or engineered material

use); PREP (Preparation); USES (Uses)

(esters; manuf. of polyoxyalkylene mercapto fatty

acid esters for prepn. of block copolymer)

IT Esterification

> (manuf. of polyoxyalkylene mercapto fatty acid esters for prepn. of block copolymer)

IT 51158-47-5P, Polyethylene glycol bis(3-mercaptopropionate)

60735-92-4P

RL: IMF (Industrial manufacture); TEM (Technical or engineered material

use); PREP (Preparation); USES (Uses)

(manuf. of polyoxyalkylene mercapto fatty acid

esters for prepn. of block copolymer)

ΙT 420120-94-1P 420120-95-2P

RL: IMF (Industrial manufacture); PREP (Preparation)

(triblock; manuf. of polyoxyalkylene mercapto fatty acid esters for prepn. of block copolymer)

51158-47-5P, Polyethylene glycol bis(3-mercaptopropionate) ΙT

RL: IMF (Industrial manufacture); TEM (Technical or engineered material

use); PREP (Preparation); USES (Uses)

(manuf. of polyoxyalkylene mercapto fatty acid esters for prepn. of block copolymer)

RN 51158-47-5 HCA

CN Poly(oxy-1, 2-ethanediyl), .alpha.-(3-mercapto-1-oxopropyl)-.omega.-(3mercapto-1-oxopropoxy) - (9CI) (CA INDEX NAME)

$$\text{HS-CH}_2\text{-CH}_2\text{-CH}_2\text{-CH}_2\text{-CH}_2\text{-CH}_2\text{-CH}_2\text{-CH}_2\text{-SH}$$

L115 ANSWER 5 OF 72 HCA COPYRIGHT 2003 ACS

132:13156 Anticorrosive coating compositions for use on metal and precoated steel surface and method for using them. Hosono, Tetsuo; Nakazato, Michiaki; Inoue, Tadayoshi (Nippon Dacro Shamrock Co., Ltd., Japan). Int. Appl. WO 9960185 A1 19991125, 62 pp. DESIGNATED STATES: W: CN, JP, KR. (Japanese). CODEN: PIXXD2. APPLICATION: WO 1999-JP2511 19990514. PRIORITY: JP 1998-133824 19980515.

The compns. which do not contain hexavalent chromium compd.-type AB pollutants, comprise the polyesters bearing .gtoreq.1 SH groups, optionally curing agents, curing catalysts or/and silica (as anti-dripping aid), and can be cured by heating. Thus, heating 1 mol ethylene glycol with 2 mol 3-mercaptopropionic acid to 180.degree. over 2 h and at 180-190.degree. for 2 h and terminating at 210-220.degree. while removing water byproduct gave a diester 100 parts of which was combined with 200 MIBK to give a coating.

ICM C23C022-00 ICS C23C022-53 IC

42-10 (Coatings, Inks, and Related Products) CC

Section cross-reference(s): 55, 56

96-27-5P 638-16-4P, 1,3,5-Triazine-2,4,6(1H,3H,5H)-trithione ΙT

7539-04-0P, Pentaerythritol tri(3-mercaptopropionate) 7539-05-1P, Pentaerythritol di (3-mercaptopropionate) 7575-23-7P, Pentaerythritol tetra(3-mercaptopropionate) 10193-99-4P, Pentaerythritol tetra(mercaptoacetate) 22504-50-3P, Ethylene glycol di(3-mercaptopropionate) 34039-24-2P, Thiomaleic acid 67905-23-1P. 33007-83-9P Trimethylolpropane mono (3-mercaptopropionate) 251635-92-4P, Ethylene glycol-terephthalic acid copolymer diester with 3-mercaptopropionic acid 251635-93-5P, Terephthalic acid-trimethylolpropane copolymer ester with 3-mercaptopropionic acid 251635-94-6P, Pentaerythritol-terephthalic acid copolymer ester with mercaptoacetic acid 251635-95-7P, Pentaerythritol-terephthalic acid copolymer ester with 3-mercaptopropionic acid 251635-96-8P, Adipic acid-pentaerythritol copolymer ester with 3-mercaptopropionic acid 251635-97-9P, Hitaloid D 1002 3-mercaptopropionate ester RL: IMF (Industrial manufacture); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (anticorrosive coating compns. for use on metal and precoated steel surface and method for using steel plate) 7539-04-0P, Pentaerythritol tri(3-mercaptopropionate) TΤ **7539-05-1P**, Pentaerythritol di(3-mercaptopropionate) 7575-23-7P, Pentaerythritol tetra(3-mercaptopropionate) 10193-99-4P, Pentaerythritol tetra(mercaptoacetate) 22504-50-3P, Ethylene glycol di (3-mercaptopropionate) 33007-83-9P RL: IMF (Industrial manufacture); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (anticorrosive coating compns. for use on metal and precoated steel surface and method for using steel plate)

RN 7539-05-1 HCA

7539-04-0 HCA

RN

CN

CN Propanoic acid, 3-mercapto-, 2,2-bis(hydroxymethyl)-1,3-propanediyl ester (9CI) (CA INDEX NAME)

Propanoic acid, 3-mercapto-, 2-(hydroxymethyl)-2-[(3-mercapto-1-

oxopropoxy)methyl]-1,3-propanediyl ester (9CI) (CA INDEX NAME)

RN 7575-23-7 HCA

CN Propanoic acid, 3-mercapto-, 2,2-bis((3-mercapto-1-oxopropoxy)methyl]-1,3-propanediyl ester (9CI) (CA INDEX NAME)

RN 10193-99-4 HCA

CN Acetic acid, mercapto-, 2,2-bis[[(mercaptoacetyl)oxy]methyl]-1,3propanediyl ester (9CI) (CA INDEX NAME)

RN 22504-50-3 HCA

CN Propanoic acid, 3-mercapto-, 1,2-ethanediyl ester (9CI) (CA INDEX NAME)

RN 33007-83-9 HCA

CN Propanoic acid, 3-mercapto-, 2-ethyl-2-[(3-mercapto-1-oxopropoxy)methyl]1,3-propanediyl ester (9CI) (CA INDEX NAME)

L115 ANSWER 10 OF 72 HCA COPYRIGHT 2003 ACS

128:193616 Rubber compositions with improved tensile properties. Kawatsa, Satoshi (Yokohama Rubber Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 10060199 A2 19980303 Heisei, 4 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1996-219941 19960821.

AB The compns., useful for hoses, tire inner liners, etc., comprise halogen-contg. C4-7-isomonoolefin-p-alkylstyrene copolymers 100, compds. having .gtoreq.2 COCH2SH 0.5-10.0, and .gtoreq.1 C12-22 (un)satd. fatty acid Zn salts and/or ZnO 1-10 parts. Thus, EXXPRO 89-4 (brominated isobutylene-p-methylstyrene copolymer) was blended with 2 phr Zn stearate and 2 phr polyoxypropylene glycerol ether

tris(thioglycolate) (I), kneaded, and press vulcanized to give a sheet showing improved tensile breaking strength and elongation compared with a control not contq. I.

TC ICM C08L023-20

ICS C08K003-20; C08K005-098; C08K005-36; C08L025-08

39-9 (Synthetic Elastomers and Natural Rubber)

9018-90-0 10193-96-1, Trimethylolpropane tris(thioglycolate) TΤ

10193-99-4, Pentaerythritol tetrakis (thioglycolate)

RL: MOA (Modifier or additive use); USES (Uses)

(vulcanizing agent; halogenated isomonoolefin-alkylstyrene rubber compns. with improved tensile properties)

10193-96-1, Trimethylolpropane tris(thioglycolate) TT

10193-99-4, Pentaerythritol tetrakis(thioglycolate)

RL: MOA (Modifier or additive use); USES (Uses)

(vulcanizing agent; halogenated isomonoolefin-alkylstyrene rubber compns. with improved tensile properties)

10193-96-1 HCA RN

CN Acetic acid, mercapto-, 2-ethyl-2-[[(mercaptoacetyl)oxy]methyl]-1,3propanediyl ester (9CI) (CA INDEX NAME)

RN 10193-99-4 HCA

Acetic acid, mercapto-, 2,2-bis[[(mercaptoacetyl)oxy]methyl]-1,3-CN propanediyl ester (9CI) (CA INDEX NAME)

L115 ANSWER 15 OF 72 HCA COPYRIGHT 2003 ACS

124:59414 Epoxy resin-containing unsaturated thermosetting resin compositions for in-mold coating. Morishita, Natsuki; Tsuji, Toshimitsu (Sekisui Chemical Co Ltd, Japan). Jpn. Kokai Tokkyo Koho JP 07242797 A2 19950919 Heisei, 17 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1994-33444 19940303.

Title compns. for coatings with improved impact resistance and adhesion AB strength contain reactive unsatd. thermosetting resins, epoxy resins, and (a) unsatd. monoamines or (b) unsatd. monocarboxylic acids or unsatd. monomercaptans. Thus, a compn. of GY 250 18, allylamine 2, styrene soln. of isophthalate-based unsatd. polyester 80, tert-butylperoxy benzoate 0.8, CaCO3 30, and TiO2 10 parts was subjected to in-mold coating on sheet-molding-compd. (SMC, polystyrene/polyester) to give a test piece showing cross-cut adhesion 100/100 and high impact resistance.

IC ICM C08L063-00

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ICS B29C039-10; B29C043-20; C08G059-40; C08G059-56
ICI B29K101-10
CC
    42-10 (Coatings, Inks, and Related Products)
    Section cross-reference(s): 38
TΤ
    79-39-ODP, Methacrylamide, reaction products with epoxy resins and unsatd.
                          79-41-4DP, reaction products with epoxy resins and
    thermosetting resins
    unsatd. thermosetting resins 100-42-5DP, Styrene, reaction products with
    vinyl-terminated polyoxyalkylenes and epoxy resins
                                                        107-11-9DP,
    Allylamine, reaction products with epoxy resins and unsatd. thermosetting
    resins
             108-31-6DP, 2,5-Furandione, reaction products with epoxy resins
    and unsatd. thermosetting resins 109-80-8DP, 1,3-Dimercaptopropane,
    reaction products with epoxy resins and unsatd. thermosetting resins
    111-40-0DP, Diethylenetriamine, reaction products with epoxy resins and
    unsatd. thermosetting resins 124-04-9DP, Hexanedioic acid,
    reaction products with epoxy resins and unsatd. thermosetting resins
    868-77-9DP, reaction products with isocyanate-terminated polyoxyalkylenes
    and epoxy resins 870-23-5DP, Allylmercaptan, reaction products with
    epoxy resins and unsatd. thermosetting resins
                                                   5954-68-7DP, reaction
    products with epoxy resins and unsatd. thermosetting resins
    10193-96-1DP, reaction products with epoxy resins and unsatd.
                          25068-38-6DP, GY 250, reaction products with
    thermosetting resins
    unsatd. resins
                     25322-68-3DP, vinyl-terminated, reaction products with
    epoxy resins 26471-62-5DP, TDI, reaction products with polyoxyalkylenes
    hydroxy-contg. vinyl compds. and epoxy resins 26590-20-5DP,
    Methyltetrahydrophthalic anhydride, reaction products with epoxy resins
    and unsatd. thermosetting resins 31305-94-9DP, MY 720, reaction products
    with unsatd. resins 61970-25-ODP, Bisphenol A-epichlorohydrin copolymer
    methacrylate, reaction products with epoxy resins and unsatd. monomers
    64859-69-4DP, EPN 1139, reaction products with unsatd. resins
                  172487-30-8P 172487-31-9P 172487-32-0P
    172487-29-5P
                                                 172487-37-5P
    172487-34-2P
                  172487-35-3P 172487-36-4P
                  172487-40-0P 172487-41-1P
                                                172487-42-2P
    172487-39-7P
    RL: IMF (Industrial manufacture); PEP (Physical, engineering or chemical
    process); POF (Polymer in formulation); TEM (Technical or engineered
    material use); PREP (Preparation); PROC (Process); USES (Uses)
        (in-mold coating using unsatd, thermosetting resins contq. epoxy
       resins)
    124-04-9DP, Hexanedioic acid, reaction products with epoxy resins
    and unsatd. thermosetting resins 10193-96-1DP, reaction products
    with epoxy resins and unsatd. thermosetting resins
    RL: IMF (Industrial manufacture); PEP (Physical, engineering or chemical
    process); POF (Polymer in formulation); TEM (Technical or engineered
    material use); PREP (Preparation); PROC (Process); USES (Uses)
        (in-mold coating using unsatd. thermosetting resins contg. epoxy
       resins)
    124-04-9 HCA
RN
CN
    Hexanedioic acid (9CI) (CA INDEX NAME)
HO2C- (CH2) 4-CO2H
```

Acetic acid, mercapto-, 2-ethyl-2-[[(mercaptoacetyl)oxy]methyl]-1,3-

propanediyl ester (9CI) (CA INDEX NAME)

10193-96-1 HCA

RN

CN

L115 ANSWER 20 OF 72 HCA COPYRIGHT 2003 ACS

121:117335 Two-component permanent-waving composition with successive diminution of the thio group effect by addition and partial neutralization. Hartmann, Peter (Hartmann-Haarkosmetik GmbH, Germany). Ger. Offen. DE 4300320 Al 19940714, 6 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1993-4300320 19930108.

AΒ The title compn. consists of (a) an aq. soln. of a keratin-reducing mercapto compd. (e.g. thioglycolic acid, glyceryl thioglycolate, cysteine, cysteamine) at pH >7.0 and (b) a sep. soln. of 0.01-20% maleic or fumaric acid or their salts and 0.01-10% capillary-active or noncapillary-active cationic compd. (pH <7). The solns. are mixed just before use in a proportion depending on the quality and condition of the hair to avoid damage to the hair from the mercapto compd. Thus, component (a) contained 50% ag. ammonium thioglycolate 27.0, NH3 1.70, perfume oil 0.2, ethoxylated nonylphenol 0.8, and water 70.3 g (pH 9.5) and component (b) contained trimethylcetylammonium chloride 1.0, coco fatty acid dimethylammonium betaine 1.0, maleic acid 4.0, ethoxylated nonylphenol 0.8, perfume oil 0.2, and water 93.0. Components (a) and (b) were mixed in proportions varying from 90:10 (final pH 9.4) for strong untreated hair to 40:60 (final pH 6.8) for very sensitive, bleached, porous hair. The decrease in reducing agent concn. after 20 min was 4 and 26%, resp., in the 2 cases.

ICM A61K007~09 IC

ICS A45D007-04

62-3 (Essential Oils and Cosmetics) CC

52-90-4, Cysteine, biological studies 60-23-1, Cysteamine 68-11-1, IT Thioglycolic acid, biological studies 79-42-5, Thiolactic acid 14974-53-9, Glyceryl thioglycolate 134367-07-0

RL: BIOL (Biological study)

(modulation of, in hair permanent-waving compns. with fumarate and maleate)

ΙT 14974-53-9, Glyceryl thioglycolate

RL: PROC (Process)

(modulation of, in hair permanent-waving compns. with fumarate and maleate)

RN 14974-53-9 HCA

Acetic acid, mercapto-, 1,2,3-propanetriyl ester (8CI, 9CI) (CA INDEX CN NAME)

L115 ANSWER 25 OF 72 HCA COPYRIGHT 2003 ACS 115:137483 Catalysts and process for curing epoxy resins and unsaturated polyesters and polyurethanes in presence of thiol compound complexes with metal salts. Giovando, Gualtiero (AKZO N. V., Neth.; Saint Peter S.r.l.). PCT Int. Appl. WO 9012826 A1 19901101, 41 pp. DESIGNATED STATES: W: CA, JP, US; RW: AT, BE, CH, DE, DK, ES, FR, GB, IT, LU, NL, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1990-EP729 19900426. PRIORITY: IT 1989-67301 19890426; IT 1989-67302 19890426; IT 1989-67954 19891107; IT 1989-68109 19891218.

AB Cocatalyst compns. for free-radical curing title polymers comprise complexes of metal (Li, Al, Mg, Mn, Zn, Sn) salts with thiols or thiol adducts with epoxides and anhydrides. Thus, to 100 g DSM NX 170 (unsatd. polyester) were added 0.5 g pentaerythritol tetrakis(mercaptoacetate)maleic anhydride adduct and 0.2 g AlCl3 in an 10% ethanolic soln. To the mixt. was added 2% 50:50 Me Et ketone peroxide/acetylacetone peroxide. This sample had time to gelation 3 min, time for exothermal peak 5 min, and temp. of exothermal peak 126.degree..

ICM C08F299-04 IC ICS C08F299-06; C08K005-37

37-6 (Plastics Manufacture and Processing) CC

57-48-7, Fructose, uses and 50-99-7, D-Glucose, uses and miscellaneous miscellaneous 77-79-2, Sulpholene 77-92-9D, Citric acid, esters with 85-42-7 85-43-8, Tetrahydrophthalic anhydride mercapto alcs. 87-69-4D, esters with mercapto alcs. 89-32-7 93-91-4, Benzovlacetone 94-36-0, Dibenzoyl peroxide, uses and miscellaneous 105-53-3, 106-87-6 107-22-2, Ethanedial 108-30-5, Succinic Diethvlmalonate anhydride, uses and miscellaneous 108-31-6, 2,5-Furandione, uses and miscellaneous 110-06-5, Di-tert-butyl disulfide 110-15-6D, Succinic acid, derivs. 110-15-6D, Succinic acid, esters with mercapto alcs. 110-16-7D, 2-Butenedioic acid (Z)-, esters with mercapto alcs. 110-17-8D, 2-Butenedioic acid (E)-, esters with mercapto alcs. Diethylene glycol, uses and miscellaneous 115-27-5, Chlorendic anhydride 120-46-7, Dibenzoylmethane 123-54-6, Acetylacetone, uses and miscellaneous 124-04-9D, Hexanedioic acid, esters with mercapto 126-33-0, Sulpholane 127-17-3D, Pyruvic acid, esters Ascorbic palmitate 141-82-2D, Malonic acid, esters with mercapto alcs. 141-97-9, Ethylacetoacetate 144-62-7D, Oxalic acid, esters with mercapto 328-50-7D, esters 431-03-8, Diacetyl 1338-23-4 1675-54-3 2180-18-9, Manganese acetate 2224-15-9 2561-85-5, Dodecylsuccinic 4720-60-9 4756-13-2, 1,2,3-Propanetrithiol 4802-20-4 6915-15-7D, Malic acid, esters with mercapto alcs. 7440-31-5D, Tin, salts, complexes 7447-41-8, Lithium chloride (LiCl), uses and miscellaneous 7575-23-7 7646-85-7, Zinc chloride, uses and 7722-84-1, Hydrogen peroxide (H2O2), uses and miscellaneous miscellaneous 10193-99-4 11138-47-9, Sodium perborate 16096-30-3, Propylene glycol diglycidyl ether 16096-31-4 17557-23-2 22504-50-3, 1,2-Ethylene glycol bis(3-mercaptopropionate) 25134-21-8, Methylnadic anhydride 25550-51-0, Methylhexahydrophthalic anhydride 26590-20-5, Methyl tetrahydrophthalic anhydride 26951-52-0 27043-36-3 27252-21-7D, Benzenetricarboxylic acid, esters with mercapto 37187-22-7 85758-64-1, Tris(mercaptoethyl)citrate 87110-76-7, Bisphenol F diglycidyl ether 135952-47-5, Sorbityl tetramercaptoacetate 135986-46-8, 1,2-Propanedithiolmaleate 136002-69-2 136013-61-1, Trimercaptomethyl citrate 136036-35-6, 1,2,6-Hexanetrithiol 136036-36-7, Tris(mercapto-2-propyl) citrate RL: CAT (Catalyst use); USES (Uses) (catalysts, for curing unsatd. polymers and epoxy resins)

124-04-9D, Hexanedioic acid, esters with mercapto alcs. 7575-23-7 10193-99-4 22504-50-3, 1,2-Ethylene

glycol bis(3-mercaptopropionate) 85758-64-1, Tris(mercaptoethyl)citrate 136002-69-2 136013-61-1, Trimercaptomethyl citrate 136036-36-7, Tris(mercapto-2-propyl) citrate RL: CAT (Catalyst use); USES (Uses) (catalysts, for curing unsatd. polymers and epoxy resins) 124~04-9 HCA RN CN Hexanedioic acid (9CI) (CA INDEX NAME)

HO2C- (CH2) 4-CO2H

RN 7575-23-7 HCA

Propanoic acid, 3-mercapto-, 2,2-bis[(3-mercapto-1-oxopropoxy)methyl]-1,3-CN propanediyl ester (9CI) (CA INDEX NAME)

RN 10193-99-4 HCA

CN Acetic acid, mercapto-, 2,2-bis[[(mercaptoacetyl)oxy]methyl]-1,3propanediyl ester (9CI) (CA INDEX NAME)

RN 22504-50-3 HCA

CN Propanoic acid, 3-mercapto-, 1,2-ethanediyl ester (9CI) (CA INDEX NAME)

85758-64-1 HCA RN

CN 1,2,3-Propanetricarboxylic acid, 2-hydroxy-, tris(2-mercaptoethyl) ester (9CI) (CA INDEX NAME)

RN 136002-69-2 HCA

CN Cyclohexanecarboxylic acid, 2,2'-[7,7-bis[[(mercaptoacetyl)oxy]methyl]-1,4,10,13-tetraoxo-5,9-dioxa-2,12-dithiatridecane-1,13-diyl|bis(methyl-(9CI) (CA INDEX NAME)

2 (D1-Me)

RN 136013-61-1 HCA

CN 1,2,3-Propanetricarboxylic acid, 2-hydroxy-, tris(mercaptomethyl) ester (9CI) (CA INDEX NAME)

RN 136036-36-7 HCA

CN 1,2,3-Propanetricarboxylic acid, 2-hydroxy-, tris(1-mercapto-1methylethyl) ester (9CI) (CA INDEX NAME)

- L115 ANSWER 30 OF 72 HCA COPYRIGHT 2003 ACS
- 109:111098 Colloidal stable vinyl halide polymerizations with mercaptan chain transfer agents. Sharaby, Zaev (Goodrich, B. F., Co., USA). Eur. Pat. Appl. EP 258832 A2 19880309, 7 pp. DESIGNATED STATES: R: BE, DE, FR, GB, IT, NL, SE. (English). CODEN: EPXXDW. APPLICATION: EP 1987-112517 19870828. PRIORITY: US 1986-902714 19860902.
- Chain transfer compns. useful for the manuf. of low mol. wt. vinyl halide AR polymer having good melt flow, particle size and distribution comprise mercapto compds. and mercaptan-miscible, water-insol. materials which are nonpolymerizable with vinyl halides such as silicones. Thus, polymg, 100 parts vinyl chloride in water in the presence of hydroxyalkyl cellulose 0.10, poly(vinyl alc.) 0.1, initiator 0.13, 2-mercaptoethanol (I) 0.5, and oligosilicone PS 340 2.5 parts gave PVC having intrinsic viscosity 0.335, av. particle size 52 .mu., and particle size distribution 24% vs. 0.68, 172, and 21, resp., for PVC prepd. without I and PS 340.
- ICM C08F014-06 ICS C08F002-38
- 35-4 (Chemistry of Synthetic High Polymers) CC
- Fatty acids, uses and miscellaneous Polyesters, uses and miscellaneous RL: USES (Uses)

(chain-transfer compn. contq., for manuf. of stable PVC colloids) 1.37 60-24-2 68-11-1, uses and miscellaneous 70-49-5 79-42-5 96-27-5

107-96-0 **123-81-9** 1338-41-6, Sorbitan monostearate 1338-43-8, Sorbitan monooleate 10047-28-6 10193-96-1 16215-21-7 19721-22-3 24980-41-4 25103-09-7 39363-95-6, Paraplex G 57 92680-71-2, Tone 0310 100359-88-4, Tone 0240 116283-76-2, Tone L

200 RL: USES (Uses)

(chain-transfer compn. contq., for manuf. of stable PVC colloids)

TT 123-81-9 10193-96-1 RL: USES (Uses)

(chain-transfer compn. contg., for manuf. of stable PVC colloids)

RN 123-81-9 HCA

Acetic acid, mercapto-, 1,2-ethanediyl ester (9CI) (CA INDEX NAME) CN

RN 10193-96-1 HCA

Acetic acid, mercapto-, 2-ethyl-2-[[(mercaptoacetyl)oxy]methyl]-1,3-CN propanediyl ester (9CI) (CA INDEX NAME)

L115 ANSWER 35 OF 72 HCA COPYRIGHT 2003 ACS

102:205540 Coating composition. Smith, Derek Hedley; Taylor, John Roberts (Ault and Wiborg Paints Ltd., UK). Eur. Pat. Appl. EP 129394 Al 19841227, 46 pp. DESIGNATED STATES: R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE.

(English). CODEN: EPXXDW. APPLICATION: EP 1984-303957 19840612. PRIORITY: GB 1983-16601 19830617.

A 2-pack, air-drying, automotive coating compn. contains an epoxy resin, AΒ an amine or amide group-contg. acrylic resin (A), and polyesters or alkyd resins contq. thiol and, optionally, carboxylic acid groups. Thus, neopentyl glycol 813, trimethylolpropane 543, and phthalic anhydride 1647 g were polymd. in N at 180.degree. for 4 h, while maintaining the reflux. and then at 200 degree. until acid value fell to 19. The reaction mixt. was cooled, admixed with 224 g mercaptoacetic acid, and heated at 200.degree. until acid value reached .apprx.24. When thinned, the resultant resin (B) had viscosity 22 P (25.degree.) and contained 70.3% nonvolatiles. A clear lacquer was formulated contg. 1489 g com. A and 139 B, as well as various additives and solvents, in the 1st package and a com, epoxy resin crosslinker in the 2nd package.

ICM C09D003-81

ICS C09D003-58; C08L063-00

ICI C08L063-00, C08L033-06, C08L101-02

42-10 (Coatings, Inks, and Related Products)

ΙT Fatty acids, esters

RL: USES (Uses)

(C9-21-branched, glycidyl esters, thiol group-contg. alkyd resins, coatings)

56-81-5D, polymers with adipic acid, pentaerythritol, phthalic anhydride, fatty acid glycidyl esters and mercaptoacetic acid 68-11-1D, esters with polyester polyols 85-44-9D, polymers with adipic acid, glycerol and pentaerythritol, esters with fatty glycidyl esters and mercaptoacetic acid 115-77-5D, polymers with adipic acid, glycerol, phthalic anhydride, fatty acid glycidyl esters and mercaptoacetic acid 124-04-9D, polymers with glycerol, pentaerythritol and phthalic anhydride, esters with fatty glycidyl esters and mercaptoacetic acid 10193-96-1D, reaction products with Bu methacrylate-Et acrylate-glycidyl methacrylate-Me methacrylate copolymer 52303-13-6D, esters with mercaptoacetic acid 78618-13-0 78618-13-0D. reaction products with trimethylyolpropane trimercaptoacetate 96387-26-7 96398-26-4

RL: TEM (Technical or engineered material use); USES (Uses) (coatings, air-drying, automotive, two-pack)

124-04-9D, polymers with glycerol, pentaerythritol and phthalic anhydride, esters with fatty glycidyl esters and mercaptoacetic acid 10193-96-1D, reaction products with Bu methacrylate-Et acrylate-glycidyl methacrylate-Me methacrylate copolymer RL: TEM (Technical or engineered material use); USES (Uses) (coatings, air-drying, automotive, two-pack)

RN 124-04-9 HCA

CN Hexanedioic acid (9CI) (CA INDEX NAME)

HO2C- (CH2) 4-CO2H

10193-96-1 HCA RN

CN Acetic acid, mercapto-, 2-ethyl-2-[[(mercaptoacetyl)oxy]methyl]-1,3propanediyl ester (9CI) (CA INDEX NAME)

L115 ANSWER 45 OF 72 HCA COPYRIGHT 2003 ACS
88:7920 Curable polyene-polymercaptan compositions. Derek, J. R. Massy;
Winterbottom, Kenneth (Ciba-Geigy A.-G., Switz.). S. African ZA 7501222
19751212, 44 pp. (English). CODEN: SFXXAB. APPLICATION: ZA 1975-1222
19740227.

GI

$$\begin{array}{c} \text{CH}_2 - \\ \text{CH} - \\ \text{CH}_2 - \\ \text{CH}_2 - \\ \end{array} \\ \text{O (CH}_2 \text{CHMeO) }_n \text{CH}_2 \text{CH (OH) CH}_2 \text{N (Bu) COCH: CHCO}_2 \text{H} \\ \text{CH}_2 - \\ \end{array} \\ \begin{array}{c} \text{CH}_2 - \\ \text{CH}$$

AB Compns. contg. maleamated reaction products (prepd. by reaction of poly(oxypropylene) ethers or linoleic dimer-trimer mixts. with mono- or polyamines and maleic anhydride) and HS group-terminated polyols or acrylonitrile-butadiene copolymers are useful in the manuf. of coatings, adhesives, foams, and castings. Thus, a mixt. contg. a CHCl3 soln. of glycerol tris[poly(oxypropylene)] triglycidyl ether [37237-76-6] of mol. wt. 1,000 and 3 molar equivs. of BuNH2 [109-73-9] was treated with 3 molar equivs. of maleic anhydride [108-31-6] in CHCl3 at <40.degree. to give a 50% CHCl3 soln. of polymaleamate (I) [61722-27-8]. I (11.0 g) was mixed with 1.0 g pentaerythritol tetrathioglycolate [10193-99-4.] and 1 ml 25% aq. Na2CO3 to give a soft, large-celled foam which was self-extinguishing.

IC C07C

CC 36-6 (Plastics Manufacture and Processing)

IT Fatty acids, polymers

(dimers and trimers, aminoamides, adducts with maleic anhydride, prepn. and crosslinking of, with polymercaptans)

IT 9018-90-0 10193-99-4 14970-87-7 31942-94-6 37286-65-0

58984-21-7

RL: MOA (Modifier or additive use); USES (Uses) (crosslinking agents, for polymaleamates)

IT 10193-99-4

RL: MOA (Modifier or additive use); USES (Uses) (crosslinking agents, for polymaleamates)

RN 10193-99-4 HCA

CN Acetic acid, mercapto-, 2,2-bis[[(mercaptoacetyl)oxy]methyl]-1,3propanediyl ester (9CI) (CA INDEX NAME)

IT 71095-72-2

RL: USES (Uses)

(primers, on fiber-reinforced plastics, for plating with copper)

RN 71095-72-2 HCA

CN Acetic acid, mercapto-, 2,2-bis[[(mercaptoacetyl)oxy]methyl]-1,3-propanediyl ester, polymer with 3,9-diethenyl-2,4,8,10-tetraoxaspiro[5.5]undecane and 2,2'-[(1-methylethylidene)bis(4,1-phenyleneoxymethylene)]bis[oxirane] (9CI) (CA INDEX NAME)

CM 1

CRN 10193-99-4 CMF C13 H20 O8 S4

CM 2

CRN 1675-54-3 CMF C21 H24 O4

CM 3

CRN 78-19-3 CMF C11 H16 O4

L115 ANSWER 40 OF 72 HCA COPYRIGHT 2003 ACS

91:92665 Surface treatment of electrically nonconducting materials. Kanehiro, Haruyuki; Takiyama, Eiichiro (Showa Highpolymer Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 54047766 19790414 Showa, 5 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1977-113297 19770922.

AB Bisphenol A diglycidyl ether-diallylidenepentaerythritol-pentaerythritol tetrathioglycolate copolymer [71095-72-2], adipic acid-ethylene glycol-pentaerythritol tetrathioglycolate-propylene glycol-tolylene diisocyanate copolymer [71110-40-2], or a similar polymer was used as a primer for chem. plating of PVC [9002-86-2] and fiber-reinforced plastics. Thus, 200 mL dioxane, 227 g 95% pentaerythritol tetrathioglycolate, and 63 g diallylidenepentaerythritol were mixed and irradiated with a high-pressure Hg lamp at 70-80.degree. to viscosity >20 P, the product was mixed with 0.3 g hydroquinone, dild. with dioxane to viscosity 2.5-3 P, and mixed with dioxane contg. bisphenol A diglycidyl ether at SH-epoxy ratio 1.5:1 to give a primer, and a fiber-reinforced plastic was sprayed with the primer and plated with Cu.

IC C08J007-04; C23C003-02

CC 37-3 (Plastics Fabrication and Uses)

IT 71095-94-8

RL: USES (Uses)

(primers, on PVC, for plating with copper)

IT 71095-72-2

RL: USES (Uses)

(primers, on fiber-reinforced plastics, for plating with copper)

IT 71095-94-8

RL: USES (Uses)

(primers, on PVC, for plating with copper)

RN 71095-94-8 HCA

CN Acetic acid, mercapto-, 2,2-bis[[(mercaptoacetyl)oxy]methyl]-1,3propanediyl ester, polymer with DEN 438 (9CI) (CA INDEX NAME)

CM 1

CRN 63957-64-2

CMF Unspecified

CCI PMS, MAN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

CRN 10193-99-4 CMF C13 H20 O8 S4

L115 ANSWER 50 OF 72 HCA COPYRIGHT 2003 ACS

84:166348 Photocurable resin lacquer. (Grace, W. R., and Co., USA). Jpn. Kokai Tokkyo Koho JP 50103536 19750815 Showa, 20 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1974-8643 19740121.

AB Photocurable lacquer compns. were prepd. from compns. contq. a polyene component having .gtoreq.2 C:C per mol., a polythiol component having .gtoreq.2 SH groups per mol., a resin component, and a photocuring catalyst. Thus, 10 parts of a polyester [32505-78-5] prepd. from a mixt. of phthalic anhydride 275, maleic anhydride 60.8, adipic acid 90.5, and diethylene glycol 328 g was mixed at 70.degree. with triallyl isocyanurate [1025-15-6] 10 pentaerythritol tetrakis(3-mercaptopropionate) [7575-23-7] 14, benzophenone 0.5, H3PO4 0.025, a com. antioxidant 0.05 g to give a transparent lacquer (viscosity 12,000-8000 cP, pH 4.5-5.5). The lacquer was coated on a red printed steel can, and exposed to uv to give a cured lacquer film.

C09D; C08F

CC 42-3 (Coatings, Inks, and Related Products)

7575-23-7

RL: TEM (Technical or engineered material use); USES (Uses) (coatings, contg. isocyanurates and polyesters, photocurable) 7575-23-7

IΤ

RL: TEM (Technical or engineered material use); USES (Uses) (coatings, contg. isocyanurates and polyesters, photocurable)

RN 7575-23-7 HCA

CN Propanoic acid, 3-mercapto-, 2,2-bis[(3-mercapto-1-oxopropoxy)methyl]-1,3propanediyl ester (9CI) (CA INDEX NAME)

L115 ANSWER 55 OF 72 HCA COPYRIGHT 2003 ACS

84:18488 Hardening of composition containing polyepoxy compound. (Dow Chemical Co., USA). Neth. Appl. NL 7314740 19750429, 11 pp. (Dutch). CODEN: NAXXAN. APPLICATION: NL 1973-14740 19731026.

Epoxy resins were hardened in presence of oxazolines, using as accelerators compds. of formula R(X)n(R = alkyl group and X = halo, CO2H,SH, n = 1-2; or R = arom. group, X = OH SH, n = 1-3). Thus, 15.4g bisphenol A-epichlorohydrin polymer [25068-38-6] and 9.6 g

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2,2'-(thiodiethylene)bis(2-oxazoline) [29633-58-7] were mixed, heated to
     120.degree. over 30 min, cooled to 90.degree. mixed with 1.0 q
     adipic acid [124-04-9], and heated to
     150.degree., giving gelation after 15 min and complete hardening in 1 hr
     to a material with tensile strength .gtoreq.770 kg/cm2. A comparison
     without the adipic acid had gel time 50 min and
     tensile strength 581 kg/cm2 after 1 hr at 150.degree..
TC.
     C08G
CC
     36-6 (Plastics Manufacture and Processing)
     epoxy resin crosslinking catalyst; adipic acid
     crosslinking catalyst; oxazoline crosslinking epoxy resin
             79-34-5 96-11-7 96-12-8 108-46-3, uses and miscellaneous
     108-73-6 108-95-2, uses and miscellaneous 111-24-0 124-04-9,
     uses and miscellaneous
                            1522-92-5 17527-79-6 22504-50-3
     RL: CAT (Catalyst use); USES (Uses)
        (catalysts, for crosslinking of epoxy resins with oxazolines)
     124-04-9, uses and miscellaneous 22504-50-3
     RL: CAT (Catalyst use); USES (Uses)
        (catalysts, for crosslinking of epoxy resins with oxazolines)
RN
     124-04-9 HCA
CN
     Hexanedioic acid (9CI) (CA INDEX NAME)
HO_2C - (CH_2)_4 - CO_2H
RN
     22504-50-3 HCA
     Propanoic acid, 3-mercapto-, 1,2-ethanediyl ester (9CI) (CA INDEX NAME)
HS-CH2-CH2-C-O-CH2-CH2-O-C-CH2-CH2-SH
L115 ANSWER 60 OF 72 HCA COPYRIGHT 2003 ACS
83:80475 Hardening of prepolymers. Tomalia, Donald A.; Thomas, Robert James
     (Dow Chemical Co., USA). Ger. DE 2355207 19750507, 17 pp. (German).
     CODEN: GWXXAW. APPLICATION: DE 1973-2355207 19731105.
    Compds. (12) such as adipic acid (I) [124-04-9
     ], 1,5-dibromopentane [111-24-0], ethylene bis(3-mercaptopropionate) [
    22504-50-3], and resorcinol [108-46-3] were used to accelerate the
    hardening of epoxy resins contg. bis[2-(2-oxazolinyl)ethyl] sulfide (II)
     [29633-58-7] or 1,4-di(2-oxazolinyl)butane [36931-59-6]. Thus, 15.4 g
    bisphenol A-epichlorohydrin copolymer [25068-38-6] (epoxy equiv. wt.
    186-192) was mixed with 9.6 g II, heated 30 min at 120.degree., mixed at
     90.degree. with 1 g I, gelled during 18 min at 150.degree., and hardened
    during 1 hr at 150.degree. to give a test specimen with tensile strength
    773 kg/cm2, compared with gel time 50 min and tensile strength 520 kg/cm2
     in the absence of I.
IC
    C08G
    36-6 (Plastics Manufacture and Processing)
CC
IT
    74-95-3 79-34-5 96-11-7 96-12-8 108-46-3, uses and miscellaneous
              108-95-2, uses and miscellaneous 111-24-0 124-04-9,
    108-73-6
    uses and miscellaneous 1522-92-5 17527-79-6 22504-50-3
    RL: CAT (Catalyst use); USES (Uses)
        (catalysts, for crosslinking of epoxy resins by oxazolines)
TT
    124-04-9, uses and miscellaneous 22504-50-3
    RL: CAT (Catalyst use); USES (Uses)
        (catalysts, for crosslinking of epoxy resins by oxazolines)
RN
    124-04-9 HCA
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Hexanedioic acid (9CI) (CA INDEX NAME)

 HO_2C^- (CH₂)₄ - CO_2H

RN 22504-50-3 HCA

Propanoic acid, 3-mercapto-, 1,2-ethanediyl ester (9CI) (CA INDEX NAME) CN

L115 ANSWER 65 OF 72 HCA COPYRIGHT 2003 ACS

78:5567 Chemically printing. Guthrie, James L.; Rendulic, Francis J. (Grace, W. R., and Co.). U.S. US 3694241 19720926, 4 pp. (English). CODEN: USXXAM. APPLICATION: US 1971-135435 19710419.

Chem. curable printing inks were prepd. from Bonadur Red (I, phthalocyanine blue, TiO2, benzidine yellow, or channel black 1-30, allyl isocyanate-poly(tetramethylene ether) diol adduct (II), or a polytetraene (prepd. from phthalic anhydride, diethylene glycol, and optionally trimethylolpropane diallyl ether, allyl alc., trimellitic anhydride, propylene glycol, and adipic acid) 30-90, pentaerythritol tetrakis(.beta.-mercaptopropionate) (III) [7575-23-7] 30-90, and 2,4,3-trimethoxybenzophenone (IV) [3770-80-7] or benzophenone [119-61-9] 0 or 0.05-5 parts/100 parts polyene-polythiol sensitizer. The inks coated on paper to give products with good hardness and gloss, and no strike-through. Thus, II 83, I 5.2, III 17, and IV 0.52 parts/100 parts polyene-polythiol combination were blended at about 80.deg.. A newsprint of quality printing paper was dipped into a 0.01-0.1% ag. FeCl3 soln., blotted, dried, and relief coated with the ink to give 2 .mu. thick images.

IC B41C; B41M; D06N

NCL 117015000

42-12 (Coatings, Inks, and Related Products) CC

7575~23-7

RL: USES (Uses)

(printing inks, contg. polydienes, pigments and sensitizers, chem.-curable)

TТ 7575-23-7

RL: USES (Uses)

(printing inks, contg. polydienes, pigments and sensitizers,

chem.-curable)

RN 7575-23-7 HCA

CN Propanoic acid, 3-mercapto-, 2,2-bis[(3-mercapto-1-oxopropoxy)methyl]-1,3propanediyl ester (9CI) (CA INDEX NAME)

L115 ANSWER 70 OF 72 HCA COPYRIGHT 2003 ACS 67:100575 Poly(thio epoxides). (CIBA Ltd.). Brit. GB 1082104 19670906, 12 pp. (English). CODEN: BRXXAA. APPLICATION: GB 19650923.

AB Poly(thio epoxides) (I) of low viscosity, which are solvent resistant and

need no plasticizer, are prepd. by treating polymercaptans with olefinically unsatd. epoxides. I possess good elec. properties such as a low dissipation factor. Thus, a reaction mixt. of 1 mole triethylene glycol, 4 moles mercaptoacetic acid (II), and 500 ml. toluene was heated from 25 to 124.degree. over 1 hr., at 124-40.degree. for 1 hr. and at 140-53. degree. for 2.5 hrs. The mixt. was freed of solvent and unreacted material by distn., reaching a pot temp. of 150. degree. / 1-2 mm. to give a thin liquid residual product of 340 g. having an equiv. wt. of 147 compared to a theoretical value of 155 and a Gardner-Holdt viscosity of A. Similarly prepd. were the reaction products of II with 1,4-butanediol, 1,1,1-trimethylolpropane (III), glycerol, 1,1,1-trimethylolethane, pentaerythritol (IV), a copolymer of allyl alc. and styrene, a hydroxylated castor oil, IV and soybean oil acid (V), III and V, bisphenol A, and a phenol-HCHO resin. Also similarly treated were .beta.-mercaptopropionic acid with III and mercaptoethanol with adipic acid. Then 224 g. glycol dimercaptoacetate (VI) and 456 g. allyl glycidyl ether (VIII) were mixed at 52.degree, the temp. being held for 8 hrs. at50-5.degree, and then raised to 93.degree. over 0.5 hr. The volatile materials were then removed by stripping to a pot temp. of 101.degree./2 mm. The resultant liquid epoxide had a Gardner-Holdt viscosity of E and an epoxide equiv. wt. of 237. In a similar manner VI was treated with 2-allylphenol, vinyl-3,4-epoxycyclohexane (VIII), and limonene monoxide (IX). In a similar manner 1,4-butanedithiol was treated with VIII, trimethylolethane mercaptoacetate with VII, trimethylolpropane tris(mercaptoacetate) (X) with a mixt. of VII and IX, X, with VIII, III-dimerized V ester-mercaptoacetate with VIII, pentaerythritol tetrakis(mercaptoacetate) (XI) with VII, and XI with glycidyl acrylate. A 20-q. mixt. was prepd. from the reaction product of VI with VII, methylbicyclo[2.2.1]-hept-5-ene-2,3-dicarboxylic anhydride, and 2,4,6-tris(dimethylaminomethyl)phenol. The mixt. was placed in an Al dish of 2-in. diam. and heated to dissolve the anhydride. The Al dish with its content was then heated 0.75 hr. at 100.degree. to give a heat-infusible tack-free product. Similar products were prepd. using other dimercaptans.

IC C07D

CC 35 (Synthetic High Polymers)

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IT
     Soybean oil
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RL: USES (Uses)

(acids, esters with mercaptoacetates of 2-ethyl-2-(hydroxymethyl)-1,3propanediol and pentaerythritol)

ΙT 90-72-2P 10193-94-9P 10193-95-0P 10193-96-1P 10193-97-2P 10193-98-3P 10193-99-4P 10194-00-0P 14974-53-9P 18271-65-3P 25119-62-4P, preparation 25134-21-8P 25300-74-7P 25300-75-8P 25300-86-1P 25302-57-2P 25323-57-3P 28930-57-6P 30938-34-2P 30938-35-3P 30941-68-5P 30941-71-0P 30941-72-1P

RL: PREP (Preparation) (prepn. of)

10193-95-0P 10193-96-1P 10193-97-2P 10193-98-3P 10193-99-4P 10194-00-0P 14974-53-9P 25300-74-7P 25300-86-1P 25302-57-2P 25323-57-3P 28930-57-6P 30938-34-2P 30938-35-3P 30941-68-5P 30941-71-0P 30941-72-1P RL: PREP (Preparation)

(prepn. of) RN 10193-95-0 HCA

CN Acetic acid, mercapto-, 1,4-butanediyl ester (9CI) (CA INDEX NAME)

RN 10193-96-1 HCA

CN Acetic acid, mercapto-, 2-ethyl-2-[[(mercaptoacetyl)oxy]methyl]-1,3-propanediyl ester (9CI) (CA INDEX NAME)

RN 10193-97-2 HCA

RN 10193-98-3 HCA

CN Acetic acid, mercapto-, 2-[[(mercaptoacetyl)oxy]methyl]-2-methyl-1,3propanediyl ester (9CI) (CA INDEX NAME)

RN 10193-99-4 HCA

CN Acetic acid, mercapto-, 2,2-bis[[(mercaptoacetyl)oxy]methyl]-1,3propanediyl ester (9CI) (CA INDEX NAME)

RN 10194-00-0 HCA

CN Hexanedioic acid, bis(2-mercaptoethyl) ester (9CI) (CA INDEX NAME)

RN 14974-53-9 HCA

John Calve, EIC - 1700, 308-4139

Acetic acid, mercapto-, 1,2,3-propanetriyl ester (8CI, 9CI) (CA INDEX

RN 25300-74-7 HCA

Acetic acid, mercapto-, ethylene ester, polymer with 3-vinyl-7-CN oxabicyclo[4.1.0]heptane (8CI) (CA INDEX NAME)

CM 1

CRN 123-81-9 CMF C6 H10 O4 S2

CM 2

CRN 106-86-5 CMF C8 H12 O

RN 25300-86-1 HCA

Acetic acid, mercapto-, ethylene ester, polymer with 1-(allyloxy)-2,3epoxypropane (8CI) (CA INDEX NAME)

CM 1

CRN 123-81-9 CMF C6 H10 O4 S2

CM 2

CRN 106-92-3 CMF C6 H10 O2

RN 25302-57-2 HCA

CN Acetic acid, mercapto-, 1,2,3-propanetriyl ester, polymer with 1-(allyloxy)-2,3-epoxypropane (8CI) (CA INDEX NAME)

CM :

CRN 14974-53-9 CMF C9 H14 O6 S3

CM 2

CRN 106-92-3 CMF C6 H10 O2

RN 25323-57-3 HCA

CN Acetic acid, mercapto-, ethylene ester, polymer with 1-(o-allylphenoxy)-2,3-epoxypropane (8CI) (CA INDEX NAME)

CM 1

CRN 4638-04-4 CMF C12 H14 O2

CM 2

CRN 123-81-9 CMF C6 H10 O4 S2

RN 28930-57-6 HCA

CN Acetic acid, mercapto-, neopentanetetrayl ester, polymer with 1-(allyloxy)-2,3-epoxypropane (8CI) (CA INDEX NAME)

CM 1

CRN 10193-99-4 CMF C13 H20 O8 S4

CM 2

CRN 106-92-3 CMF C6 H10 O2

RN 30938-34-2 HCA

Acetic acid, mercapto-, ethylene ester, polymer with 1,2-epoxy-p-menth-8-ene (8CI) (CA INDEX NAME)

CM 1

CN

CRN 1195-92-2 CMF C10 H16 O

CM 2

CRN 123-81-9 CMF C6 H10 O4 S2

RN 30938-35-3 HCA

Acetic acid, mercapto-, triester with 2-(hydroxymethyl)-2-methyl-1,3-CN propanediol, polymer with 1-(allyloxy)-2,3-epoxypropane (8CI) (CA INDEX

CM 1

CRN 10193-98-3 CMF C11 H18 O6 S3

CM 2

CRN 106-92-3 CMF C6 H10 O2

RN 30941-68-5 HCA

CN Propionic acid, 3-mercapto-, triester with 2-(hydroxymethyl)-2-methyl-1,3propanediol, polymer with 3-vinyl-7-oxabicyclo[4.1.0]heptane (8CI) (CA INDEX NAME)

CM 1

CRN 10312-58-0 CMF C14 H24 O6 S3

CM 2

CRN 106-86-5 CMF C8 H12 O

RN 30941-71-0 HCA

CN Acrylic acid, 2,3-epoxypropyl ester, polymer with neopentanetetrayl tetrakis (mercaptoacetate) (8CI) (CA INDEX NAME)

CM 1

CRN 10193-99-4 CMF C13 H20 O8 S4

2 CM

CRN 106-90-1 CMF C6 H8 O3

RN 30941-72-1 HCA

CN Acetic acid, mercapto-, triester with 2-(hydroxymethyl)-2-methyl-1,3propanediol, polymer with 1,2-epoxy-p-menth-8-ene and 3-vinyl-7oxabicyclo[4.1.0]heptane (8CI) (CA INDEX NAME)

CM 1

CRN 10193-98-3 CMF C11 H18 O6 S3

CM 2 CRN 1195-92-2 CMF C10 H16 O

CM 3

CRN 106-86-5 CMF C8 H12 O

L115 ANSWER 71 OF 72 HCA COPYRIGHT 2003 ACS
66:29581 Curing epoxy resins and polyhydric alcohols. (CIBA Ltd.). Brit. GB
1050095 19661207, 7 pp. (English). CODEN: BRXXAA. PRIORITY: US
19620604.

A mixt. of 1 mole triethylene glycol, 4 moles HSCG2CO2H, and 500 ml. PhMe AB was heated from 25.degree. to 124.degree. during 1 hr., at 124-40.degree. for 1 hr., and at 140-53.degree. for 2.5 hrs. Distn. of the mixt. gave 340 q. triethylene glycol bis(mercaptoacetate) (I). Similarly prepd. were 1,4-butanediol bis-(mercaptoacetate) (II), 1,1,1-trimethylopropane tris(mercaptopropionate), (III), 1,1,1-trimethylolpropane tris(mercaptopropionate), glycerol mercaptoacetate, 1,1,1trimethylolethane tris-(mercaptoacetate) (IV), pentaerythritol tetrakis(mercaptoacetate) (V), styrene-allyl alc. copolymer mercaptoacetate (VI), hydroxlyated castor oil (5 OH/mole) mercaptoacetate, and mercaptoethanyl adipate (VII) from mercaptoethanol and adipic acid. A mixt. of 685 g. distd. soybean oil acids, 259 g. pentaerythritol, and sufficient PhMe for const. reflux at 220.degree. was refluxed at 220.degree. for 3 hrs., dild. with 500 ml. PhMe to cool the mixt. to 100.degree., and filtered. The filtrate was heated with 3.5 moles HSCH2CO2H at 112-21.degree. for 1 hr., at 121-144.degree. for 1 hr., and at 144-46.degree. for 3.75 hrs. Removal of the solvent gave a mixed ester of pentaerythritol with HSCH2CO2H and soybean oil acids. A mixed ester (VIII) of 1,1,1-trimethylolpropane with HSCH2CO2H and dimerized soybean oil acids was prepd. similarly. Epon 828 (an epoxy resin) was cured by heating with maleic anhydride (IX) and an ester prepd. such as I, II, III, IV, V, or VI. The mixts. became solids on heating at 75.degree. for 1 hr. and remained hard on addnl. heating at 100.degree. for hr., at 125.degree. for 1 hr., at 150.degree. for 1 hr., and at 200.degree. for 1 hr. Curing was also effected by heating a thin layer of the curing mixt. to give tack-free solid casting. The cured resins had dielec. consts. comparable to uncured resins and better dissipation factors, and were solvant resistant. A polydric alc. was prepd. from 300 g. dimerized soybean oil acids and 134 g. 1,1,1-trimethylolpropane. The polyhydric alc. 21, VIII 30, and IX 9.8 parts were cast in a Al dish

IC

CC

TT

TΤ

ΙT

ΤТ

IΤ

ΙT

RN CN

RN CN

RN

RN

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in 0.5-in. thickness and cured at 100.degree. and 150.degree. for 1 hr. at
     each temp. to give a tack-free, infusible, flexible, resin. A mixt. of
     III 14, 1,1,1-trimethylopropane 4.4, and itaconic anhydride 11 parts was
     cured similarly.
     C08G
     36 (Plastics Manufacture and Processing)
     EPOXY-POLYALC MIXTS CURING; CURING EPOXY-POLYALC MIXTS; SOYBEAN
ST
     OIL ACIDS ESTERS; MERCAPTOACETATES; POLYALC-EPOXY MIXTS CURING
     Soybean oil
     RL: USES (Uses)
        (fatty acids of, polymercapto esters from
        mercaptoacetic acid, pentaerythritol and, as crosslinking agent for
        epoxy resins and polyhydric alcs.)
     Fatty acids, uses and miscellaneous
     RL: USES (Uses)
        (polymercapto esters from mercaptoacetic acid, pentaerythritol and, as
        crosslinking agents for epoxy resins and polyhydric alcs.)
     Acetic acid, mercapto-, polymercapto esters from fatty
        acids, pentaerythritol and, uses and miscellaneous
     RL: USES (Uses)
        (as crosslinking agents for epoxy resins and polyhydric alcs.)
     Pentaerythritol, polymercapto esters from fatty acids,
        uses and miscellaneous
     RL: USES (Uses)
        (mercaptoacetic acid and, as crosslinking agents for epoxy resins and
        polyhydric alcs.)
     10193-94-9 10193-95-0 10193-96-1 10193-97-2
     10193-98-3 10193-99-4 10194-00-0
     14974-53-9
     RL: USES (Uses)
        (crosslinking of epoxy resins by dicarboxylic acid anhydrides and)
     10193-95-0 10193-96-1 10193-97-2
     10193-98-3 10193-99-4 10194-00-0
     14974-53-9
     RL: USES (Uses)
        (crosslinking of epoxy resins by dicarboxylic acid anhydrides and)
    Acetic acid, mercapto-, 1,4-butanediyl ester (9CI) (CA INDEX NAME)
HS-CH2-C-O-(CH2)4-O-C-CH2-SH
    Acetic acid, mercapto-, 2-ethyl-2-[[(mercaptoacetyl)oxy]methyl]-1,3-
    propanediyl ester (9CI) (CA INDEX NAME)
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10193-98-3 HCA

10193-97-2 HCA

Acetic acid, mercapto-, 2-[[(mercaptoacetyl)oxy]methyl]-2-methyl-1,3-

John Calve, EIC - 1700, 308-4139

propanediyl ester (9CI) (CA INDEX NAME)

RN 10193-99-4 HCA

CN Acetic acid, mercapto-, 2,2-bis[[(mercaptoacetyl)oxy]methyl]-1,3propanediyl ester (9CI) (CA INDEX NAME)

RN 10194-00-0 HCA

CN Hexanedioic acid, bis(2-mercaptoethyl) ester (9CI) (CA INDEX NAME)

RN 14974-53-9 HCA

CN Acetic acid, mercapto-, 1,2,3-propanetriyl ester (8CI, 9CI) (CA INDEX NAME)

L115 ANSWER 72 OF 72 HCA COPYRIGHT 2003 ACS 63:89820 Original Reference No. 63:16560f-g Molding and curing of epoxy-resin articles. (National Cash Register Co). NJ 6405920 19641130, 10 pp. (Unavailable). PRIORITY US 19630529

About 100 parts of a liquid epichlorohydrin-bisphenol A epoxy resin compn. with an epoxy equiv. of 175-195 and a kinematic viscosity of 5-7 poises at 25.degree.; 20 parts of an alignatic amine curing agent with a viscosity of 500 cp. at 25.degree., d23 1.05, ignition temp. (Cleveland open cup) 177.degree.; and 20 parts Mg silicate of particle size 12 .mu. were homogenized. Thirty g. of this mixt. was placed in a dielec. heater and heated for 15 min., raising the temp. to 46.1.degree.. The mixt. was poured into a preheated mold at 66.6.degree and kept for 20 min. at this

John Calve, EIC - 1700, 308-4139 Page 89

temp. The article was removed from the mold and cured for 1 hr. at 66.6.degree.. It contained no bubbles. A low-mol.-wt. fatty acid polymer, the tris(.alpha.-ethylcaproate) of tris(dimethylaminomethyl)phenol, and ethylene bis(thioqlycolate) also can be used as curing agents. IC C08G CC 48 (Plastics Technology) ΙT 123-81-9, Ethylene glycol, bis(mercaptoacetate) 4572-95-6, Hexanoic acid, 2-ethyl-, compd with .alpha., .alpha.', .alpha.''tris(dimethylamino)mesitol (3:1) (as curing agent for epoxy resin molding compns. of diglycidyl ether of bisphenol A) 123-81-9, Ethylene glycol, bis(mercaptoacetate) (as curing agent for epoxy resin molding compns. of diglycidyl ether of bisphenol A) RN 123-81-9 HCA Acetic acid, mercapto-, 1,2-ethanediyl ester (9CI) (CA INDEX NAME)